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(54) Title: **ISOPENICILLIN N SYNTHETASE AND DEACETOXYCEPHALOSPORIN C SYNTHETASE ENZYMES AND METHOD**

## (57) Abstract

A three-dimensional structure is described of a complex of isopenicillin N synthase (IPNS) with Fe and its substrate ACV. This structure is used to design modified enzymes IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, which modified enzymes may accept unnatural substrates or improve production efficiency or produce improved products. Specific modifications of specific amino acid residues are proposed and exemplified.

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## ISOPENICILLIN N SYNTHETASE AND DEACETOXYCEPHALOSPORIN C SYNTHETASE ENZYMES AND METHOD

5     Introduction

All commercially used penicillin and cephalosporin antibiotics and their derivatives are produced from fermentation derived materials containing a  $\beta$ -lactam ring. A range of organisms, including both prokaryotes and eukaryotes, and conditions may be used for their 10 fermentation. Some are produced directly by fermentation followed by isolation. Others are produced by modification of materials produced by fermentation. Commercially used cephalosporins (also known as cephems) may be produced by modification of either fermentation derived penicillins or cephalosporins.

15       The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and involves the following steps (Scheme 1):

1.       Three amino acids ( $L$ - $\alpha$ -amino adipic acid,  $L$ -cysteine,  $L$ -valine) are condensed to form a tripeptide:  $L$ - $\delta$ - $\alpha$ -amino adipoyl- $L$ -cysteinyl- $D$ -valine (ACV). During this process the  $L$ -valinyl residue is 20 converted to a  $D$ -valinyl residue. This process is catalysed *in vivo* by the enzyme ACV synthetase and is common to both penicillin and cephalosporin biosynthesis.
2.       ACV is converted to isopenicillin N in a step catalysed by the 25 enzyme isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
3.       In some organisms (e.g. *Penicillium chrysogenum* and *Aspergillus nidulans*) isopenicillin N is converted by exchange of its  $L$ - $\delta$ - $\alpha$ -amino adipoyl side chain to penicillins with other side chains, which are 30 normally more hydrophobic than the side chain of isopenicillin N. This

conversion may be catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins 5 may be commercially produced by fermentation under the appropriate conditions.

4. In some organisms (e.g. *Streptomyces clavuligerus* and *Cephalosporium acremonium*) isopenicillin N is epimerised to penicillin N. This reaction is catalysed by an epimerase enzyme.
- 10 5. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) penicillin N is converted to deacetoxycephalosporin C (DAOC). This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. *Streptomyces clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others 15 (e.g. *C. acremonium*).
6. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin 20 C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp.* DAC may be converted to cephalexin C. The genes encoding for each of the enzymes catalysing 25 steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins, their biosynthetic intermediates, and their derivatives may be of use as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or 30 intermediates used in the preparation of cephalosporins, e.g. penicillins

(including, but not exclusively, penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, e.g. Cefachlor (Scheme 2).

For reviews see J. E. Baldwin and C. J. Schofield, in 'The Chemistry of  $\beta$ -lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Aharonowitz *et al*, Ann. Rev. Microbiol., 1992, 46, 461; Cooper, Bioorg. Med. Chem., 1993, 1, 1; Baldwin and Abraham, Nat. Prod. Report., 1989, 5, 129; Baldwin, J. Heterocyclic. Chem., 1990, 27, 91.

10 **Summary of Invention**

This invention is based on our determination of the three-dimensional structure of IPNS. That the structure of IPNS complexed to manganese has been determined, was reported by some of us in Nature, Volume 375, 22 June 1995, pages 700-704. That publication did not include the co-ordinates of the individual amino acid residues, and these are now provided. Scheme 2 of that paper contains the amino acid sequence of IPNS, and also DACS, DAOCS and DAOC/DACS and other structurally related enzymes, each of which is published in Swissprot or Genbank or other database.

20 We have now determined the structure of a complex of IPNS with Fe and ACV which is a substrate for the enzyme (see Scheme 1). In solution it is this complex, and not the IPNS-Mn complex, that is actually formed during step 2 of the biosynthesis of bicyclic  $\beta$ -lactams. Because the amino acid sequences of DAOCS, DAOC/DACS, DACS and other 25 oxidases and oxygenases are so similar to that of IPNS, it is reasonable to expect that the structures of those enzymes are at least similar to that of IPNS.

We have also determined the structures of complexes of IPNS with Fe and with various analogues of ACV (in which another amino 30 acid replaced L-valine), specifically AC glycine, AC aminobutyrate, AC

alanine and AC proparglyglycine. These structures have been determined in the absence and in the presence of nitrous oxide NO. Exposure of these complexes to dioxygen alters the structures, and these altered structures have also been determined by us. From information given 5 herein about the IPNS-Fe-ACV complex, a skilled reader is able to make and characterise the other complexes referred to in this paragraph, so structural details of those other complexes are not given herein.

Thus in one aspect the invention provides Isopenicillin N synthase (IPNS) in the form of: a complex with Mn having a structure 10 designated by the X-ray co-ordinates in Table 2; or a complex with Fe and its substrate, said complex having a structure designated by the X-ray co-ordinates in Table 3.

In another aspect the invention provides Isopenicillin N synthase (IPNS) in the form of: a complex with Fe and an analogue of its 15 substrate, either in the absence or in the presence of nitrous oxide or dioxygen, said complex having a structure designated by X-ray co-ordinates analogous to that set out in Table 3.

An analogue of an IPNS substrate is a substrate oxidised by IPNS to give preferably (but not exclusively) a bicyclic compound 20 containing a  $\beta$ -lactam ring.

Table 2 sets out co-ordinates of individual amino acid residues in a crystalline complex of IPNS with manganese.

Table 3 sets out co-ordinates of individual amino acid residues in a crystalline complex of IPNS with Fe and ACV.

25 Knowledge, derived from the X-ray co-ordinates, of the three-dimensional structures of this family of related enzymes permits a skilled worker to identify specific amino acids that might be changed in order to alter or improve the properties of the enzyme in some way. While it is not possible from 3D structural information alone to predict that a specific 30 amino acid mutation will produce a specific change in the properties of the

enzyme, it is possible to identify a rather small number of amino acid residues where modification may be expected to change/improve the properties of the enzyme. The problem of identifying useful amino acid mutations is thus reduced to a level where it can readily be tackled by 5 routine screening procedures.

Thus in one aspect the invention provides use of the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOCS/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for the modification of a second 10 selected from IPNS, DAOCS, DACS, DAOCS/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway.

The three dimensional structure of a first enzyme may be the three dimensional structure of the IPNS-Fe-substrate complex referred to above. It may, however, also be that of DAOCS, DACS, DAOC/DACS or 15 another oxygenase/oxidase related by sequence or structure (e.g. 1-aminocylopropane-1-carboxylic acid oxidase) to any of IPNS, DAOCS, DACS or DAOC/DACS. The structure of the IPNS-Fe-ACV complex may be derived from two or more crystalline polymorphs, all of which are envisaged. The structure may alternatively be of the enzyme in free form 20 or in the form of some other complex such as with Mn, or with other Fe or ACV analogues, or enzyme inhibitors, or other enzyme modifiers. Preferably the second enzyme is the same as the first enzyme e.g. the 3D structure of IPNS is used as a basis for modifying IPNS. Alternatively the 3D structure of one first enzyme may be used as a basis for modifying a 25 second structurally related enzyme.

Central to the elucidation of the structure of crystalline proteins is the discovery of conditions for the production of crystals with diffract X-rays to a sufficiently high resolution. Since the cofactors (e.g. Fe(II)) and substrates (e.g. ACV) of the family of enzymes to which IPNS, 30 DAOCS, DACS, etc. belong are sensitive to modification by reaction with

dioxygen, the crystallisation of these enzymes is preferably carried out under an anaerobic atmosphere or one containing only a very low concentration of dioxygen.

The modified enzyme(s) may be used *in vitro* or introduced 5 via recombinant molecular biology techniques into an organism so that new materials can be fermented. It is recognised that multiple modifications may have to be made to an enzyme in order to change its substrate/product selectivity, and/or improve its efficiency. It is recognised that more than one modified enzyme may be used to effect the desired 10 transformation. It is recognised that in order to change the nature of the enzyme-substrate/intermediate/product interactions at a particular enzyme-substrate/intermediate interface modifications may be made to the enzyme either immediately at the interface or away from it. It is recognised that the modifications may result in hybrid enzymes containing sequences from, 15 e.g. IPNS and DAOCS or IPNS and DACS or any combination of IPNS, DAOCS, DACS or DAOCS/DACS or other related enzymes. It is also recognised that it may be desirable to further modify the organism in which the modified enzyme is to be introduced, e.g. by blocking a particular pathway in that organism (using the techniques of molecular biology) in 20 order to modify flux through the desired/modified pathway, by introducing other enzyme activities, or by other modifications. The organism into which the modified enzyme will be used may or may not contain parts of the penicillin and cephalosporin biosynthetic machinery. The organism may already have been modified to optimise or minimise production of particular 25 products or consumption of particular nutrients. More than one modified enzyme may be used in conjunction either *in vitro* or *in vivo* in an organism for the production of desirable products.

While modifications for numerous specific purposes are discussed below, it is possible to say in general that useful modifications 30 will be of three kinds:

- Those which permit the enzyme to accept unnatural substrates [i.e. substrates not normally present in the organism (which may or may not be an organism in which the enzyme is naturally occurring) in which the enzyme is operating] for the preparation of new or commercially valuable anti-bacterial materials or intermediates for the production of pharmaceutical products;
- Those which enable the enzyme to produce unnatural products [i.e. products not naturally produced in the organism in which the enzyme is operating, including 3-exomethylene cephams and 10 cephalosporins with hydrophobic side chains at the C-7 position such as phenylacetamido or phenoxyacetamido, or other unnatural side chains such as adipoyl] or improve the production of natural products of commercial value.
- Those which enhance the ability of the enzyme to produce useful products. For example DAOCS is known to catalyse the production 15 of phenylacetylcephalosporin C from penicillin G (Baldwin *et al.*, Proceedings of the 7<sup>th</sup> International Symposium on the genetics of Industrial Micro-organisms, Abstract, p262, 1994). However, this conversion is much less efficient than the DAOCS catalysed conversion of 20 penicillin N to DAOC. Modifications made to DAOCS may increase the efficiency of its catalytic conversion to penicillin G.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus 25 structural similarity with IPNS. Thus, structures of these enzymes may be predicted on the basis of the IPNS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of IPNS. Previous sequence comparisons (Roach *et al.*, *Nature*, 1995, 375, 700), using pairwise comparisons of the sequences followed by 30 single linkage cluster analysis show that IPNS, DAOCS, DACS and

DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, *J. Mol. Biol.*, 1987, **198**, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, *Methods in Enzymol.*, 1990, **183**, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physico-chemical properties (Barton and Sternberg, *J. Mol. Biol.*, 1987, **198**, 327).

5 Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DAOCS, DACS or DAOC/DACS) from another (e.g. IPNS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are largely or wholly conserved, differences in the structures of the two enzymes may 10 result from the side chains of the amino acids forming the secondary structural elements. These differences, which may alter the substrate/product selectivities of the compared enzymes, may be predictable if the three dimensional structure of one of the enzymes is 15 known. An example: the natural substrate for IPNS, ACV, has an L-configured amino adipoyl side chain, whereas the substrates for DAOCS, DACS and DAOC/DACS, i.e. penicillin N and DAOC, have D-configured 20 amino adipoyl side chains. This difference in selectivity may result from the different arrangement of amino acid side chain binding sites between IPNS and DAOCS, DACS, and DAOC/DACS. Further, it is recognised that there 25 may be significant variations between enzymes which show significant sequence/structural similarity (i.e. with standard deviation scores >5.0) in exterior regions of the enzymes, e.g. in loops and at the N- and C- termini. The relative importance of these regions in substrate binding may be 30 predicted by comparison with a known crystal structure of an enzyme with significant sequence similarity.

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In one aspect, at least one of the following amino acid residues is modified:

R287; R87; R88; Y189; S183; Y91; F285; Q330; T331; V185; L106; C104; V217; L324; L317; I325; L321; S210.

5 The residue numbering herein is taken from the paper *Nature*, 1995, 375, 700-704 referred to above. These modifications are expected to have an effect on side chain substituents at the 6-position of the penicillin molecule, or the 7-position of the cephalosporin molecule. In each case, the stated amino acid residue may be replaced by the residue 10 of any other amino acid. But in order to change the selectivity of the enzyme to accept substrates with hydrophilic or neutral side chains, the replacement is preferably to make the side chain binding pocket more hydrophobic.

15 In another aspect at least one of the following amino acid residues is modified:

V272; L231; L223; P283; T221; F211; F285; Q330; I187; V185; Y189; R279; S281; N230; Q225; N252; S210.

These modifications are expected to be associated with changes in the ring structure of the penicillin/cephalosporin molecule.

20 There follow examples of specific changes envisaged as a result of these modifications.

a) The structure of IPNS is modified in its active site region to accept unnatural substrates to produce penicillins or other bicyclic  $\beta$ -lactams of commercial use with hydrophobic side chains (Scheme 5).  
25 The process may include the following modifications (other modifications based on the use of the crystal structure of IPNS are not excluded):

Note, R87F/A/G/V/L/I/T/W/M/C/N/Q/P/S/T/E/D/R/K/H  
30 indicates that residue arginine-87, using the *Aspergillus nidulans* IPNS numbering scheme is modified to phenylalanine or alanine etc. See Roach *et al* *Nature*, 1995, 375, 700-704. ).

- 10 -

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/Y  
Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R  
S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
5 Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y  
T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
V185F/A/G/L/I/W/T/M/C/N/P/S/E/D/R/K/H/Q/Y  
10 L106F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
C104F/A/G/V/L/I/T/W/M/N/P/S/E/D/R/K/H/Q/Y  
V217F/A/G/L/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
L324F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
L317F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
15 I325F/A/G/V/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
L321F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

Note in these and in subsequently proposed modifications the  
20 amino acid residue numbering scheme is based upon that used for  
*A. nidulans* IPNS and the sequence alignments in Roach *et al* Nature,  
1995, 375, 700-704, e.g. arginine-87 in IPNS remains named as arginine-  
87 for other aligned enzymes.

It is recognised that modifications to the side chain binding  
25 interactions and the valinyl binding interactions of IPNS may have to be  
made in conjunction with each other or with other modifications in order to  
produce a useful catalyst with the desired properties. Other modifications  
based on the use of the three dimensional structures of IPNS, DACS,  
DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of  
30 these enzymes to their substrates, intermediates, modifiers, products or

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inhibitors are not excluded.

5 b) The structure of IPNS is modified in its active site region to accept natural or unnatural substrates to produce bicyclic  $\beta$ -lactams other than penicillins of commercial use (Scheme 6). For example the region of IPNS interacting with the valinyl residue of ACV may be modified such that IPNS produces 3-exomethylenecephams from ACV or other substrates for IPNS. The process may include the following modifications.

10 V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
P283F/A/G/V/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y  
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
F211A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
15 F285A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
Q330F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y  
I187F/A/G/L/W/T/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
V185F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
Y189F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q  
20 R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y  
S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y  
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y  
Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y  
N252F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y  
25 S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

30 It is recognised that modifications may have to be made in conjunction with each other or with other modifications to IPNS in order to produce a useful catalyst with the desired properties. Other modifications

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based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

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c) The side chain binding interactions of IPNS are modified such that 6-aminopenicillins or other bicyclic  $\beta$ -lactams may be produced *in vitro* or *in vivo* from dipeptides, such as cysteinyl-valine or other dipeptides (Scheme 7). Dipeptides may be produced (either *in vitro* or *in vivo*) by the 10 use of a peptide synthetase enzyme, such as ACV synthetase (which may be modified by mutagenesis or other techniques to optimise dipeptide production) or by chemical synthesis. The process may include the following modifications:

15

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R

S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y

Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R

20

F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y

Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y

T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y

V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L106F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

25

C104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y

V217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

I325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

30

L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

- 13 -

S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to 5 produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

10

d) The side chain binding interactions of IPNS are modified such that penams without any substituent at the 6-position or other bicyclic  $\beta$ -lactams, without any substituent at the 6-position, may be produced *in vitro* or *in vivo* from dipeptides or amide substrates, such as 15 3-mercaptopropionyl-valine or other dipeptides or amides (Scheme 8). The dipeptides or amides may be produced (either *in vitro* or *in vivo*) by the use of a peptide synthetase enzyme, such as ACV synthetase (which may be modified by mutagenesis or other techniques to optimise dipeptide production) or by chemical synthesis. The process may include the 20 following modifications:

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R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R  
S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y  
T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

30

- 14 -

L106F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
C104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y  
V217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
5 L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
I325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

10 It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of 15 these enzymes to their substrates, intermediates, products, modifiers, or inhibitors are not excluded.

e) 20 IPNS is modified to produce 3-exomethylenecephams with hydrophobic or other unnatural side chains (Scheme 9) (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor. The process will involve modification of both the side chain binding interactions of IPNS substrates and of the valine binding interactions and may involve the use of ACV as a substrate or the use of other unnatural substrates. The process may include the following 25 modifications, which may be made in conjunction with each other:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R  
30 S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y

- 15 -

Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y  
T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
5 V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L106F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
C104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y  
V217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
10 L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
I325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
15 L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
P283F/A/G/V/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y  
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
F211A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
I187F/A/G/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V  
20 V185F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
Y189F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q  
R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y  
S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y  
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y  
25 Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y  
N252F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y  
S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that these modifications may have to be  
30 made in conjunction with each other or with other modifications in order to

produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or 5 inhibitors are not excluded. The use of a modified IPNS in conjunction with another modified or unmodified oxygenase enzyme (e.g. DAOCS, DACS, DAOC/DACS) is not excluded.

f) The structure of DAOCS is modified in its active interactions 10 region to accept substrates (*i.e.* penicillins with hydrophobic side chains, (including, but not exclusively, penicillin G and penicillin V) to produce cephalosporins or other bicyclic  $\beta$ -lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 10). The process may include the following modifications:

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R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

20

C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S

T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y

F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y

A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q

25

P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y

T104F/A/G/V/L/I/T/W/M/N/P/S/E/D/R/K/H/Q/Y

M217F/A/G/L/I/T/W/C/N/P/S/E/D/R/K/H/Q/Y/V

I324F/A/G/V/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/L

I317F/A/G/V/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y

30

R325F/A/G/V/L/T/W/M/C/N/P/S/E/D/K/H/Q/Y/I

Y321F/A/G/V/I/T/W/M/C/N/P/S/E/D/K/H/Q/R/L

- 17 -

R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be  
5 made in conjunction with each other or with other modifications in order to  
produce a useful catalyst with the desired properties. Other modifications  
based on the use of the three dimensional structure of IPNS, DACS,  
DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of  
these enzymes to their substrates, intermediates, modifiers, products or  
10 inhibitors are not excluded.

g) The structure of DAOCS is modified in its active interactions  
region to accept natural or unnatural substrates (including, but not  
exclusively, penicillin N, isopenicillin N, adipoyl penicillin) to produce  
15 bicyclic  $\beta$ -lactams other than cephalosporins of commercial use. For  
example the region of DAOCS interacting with the thiazolidine ring of its  
natural substrate penicillin N may be modified such that the modified  
DAOCS produces 3-exomethylenecephams from penicillin N, penicillin G,  
or penicillin V, or other substrates for DAOCS (Scheme 11). The process  
20 may include the following modifications:

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

25 V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P

T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y

M211F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/N

P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/N

30 F189A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

- 18 -

R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y

S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y

N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y

Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y

5

F252F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y

R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be

10 made in conjunction with each other or with other modifications to DAOCS in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, 15 products or inhibitors are not excluded.

20 h) The side chain binding interactions of DAOCS are modified such that 6-aminopenicillins or other bicyclic  $\beta$ -lactams may be produced *in vitro* or *in vivo* from 6-amino penicillins, such as 6-aminopenicillanic acid (Scheme 12). The process may include the following modifications (other 25 modifications based on the use of the three dimensional structures of IPNS or DAOCS or DAOCS/DACS are not excluded):

25 R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S

T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y

30

F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y

- 19 -

A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
P185F/A/G/L/V/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
M217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
5 I324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
I317F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/I  
R325F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I  
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q  
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S  
10 R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, 15 DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

20 i) The side chain binding interactions of DAOCS is modified such that cephams or cephalosporins without any substituent at the 7-position or other bicyclic  $\beta$ -lactams, without any substituent at the 7-position, may be produced *in vitro* or *in vivo* from penicillins or cepham substrates (Scheme 13). The penicillanic acid may be produced whether *in vitro* or *in vivo*. The process may include the following modifications:  
25

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
30 F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

- 20 -

C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S  
T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
5 P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
T104F/A/G/V/L/I/W/M/N/C/P/S/E/D/R/K/H/Q/Y  
M217F/A/G/L/I/V/W/C/N/P/S/T/E/D/R/K/H/Q/Y  
I324F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
I317F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
10 R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I  
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q  
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S  
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

15 It is recognised that the modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of 20 these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

j) DAOCS is modified to produce 3-exomethylenecephams with hydrophobic side chains (Scheme 14) (or other intermediates for use in the 25 preparation of cephalosporin antibiotics, e.g. Cefachlor.) The process will involve modification of both the side chain binding interactions of DAOCS substrates and of the thiaxolidine binding interactions and may involve the use of penicillins with hydrophobic side chains (e.g. penicillin G or V) as substrates or the use of other unnatural substrates. The process may 30 include the following modifications (other modifications based on the use of

the three dimensional structures of IPNS or DAOCS or DAOCS/DACS are not excluded):

|    |  |
|----|--|
| 5  | V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y<br>L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y<br>L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y<br>V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P<br>T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y<br>M211A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F   |
| 10 | L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/N<br>P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/N<br>F189A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y<br>R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y<br>S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y<br>N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y |
| 15 | Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y<br>F252A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y<br>R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y<br>R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y<br>R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y<br>C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S     |
| 20 | T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y<br>F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y<br>A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q<br>P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y<br>T104F/A/G/V/L/I/N/M/N/P/S/T/E/D/R/K/H/Q/Y   |
| 25 | M217F/A/G/L/I/V/W/C/N/P/S/T/E/D/R/K/H/Q/Y<br>I324F/A/G/L/V/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y<br>I317F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y<br>R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I   |
| 30 |  |

Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L  
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S  
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

5 It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of 10 these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

15 k) The structure of DACS is modified in its active site region to accept substrates with hydrophobic side chains, including, but not exclusively, penicillin N, penicillin G and penicillin V) to produce 20 cephalosporins or other bicyclic  $\beta$ -lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 15) . The process may include the following modifications:

25 R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S  
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C  
30 L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

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R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I

Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L

R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

5

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS,  
10 DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

15 I) The structure of DACS is modified in its active site region to accept natural or unnatural substrates (including, but not exclusively, penicillin N, adipoyl penicillin) to produce bicyclic  $\beta$ -lactams other than cephalosporins of commercial use (Scheme 16). For example the region of DAOCS interacting with the thiazolidine ring of its natural substrate penicillin N may be modified such that the modified DAOCS produces 3-  
20 exomethylenecephams from penicillin N, penicillin G, or penicillin V, or other substrates for DAOCS. The process may include the following modifications

25 V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P

T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y

M211A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F

30 L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V

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P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/N  
R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y  
S281F/A/G/V/I/L/W/M/N/C/N/P/T/E/D/R/K/H/Q/Y  
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y  
5 Q225F/A/G/V/I/L/W/M/N/C/N/P/S/T/E/D/R/K/H/Y  
F252F/A/G/V/I/L/W/M/N/C/P/S/T/E/D/R/K/H/Q/Y  
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be  
10 made in conjunction with each other or with other modifications in order to  
produce a useful catalyst with the desired properties. Other modifications  
based on the use of the three dimensional structure of IPNS, DACS,  
DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of  
these enzymes to their substrates, intermediates, modifiers, products or  
15 inhibitors are not excluded.

m) The side chain binding interactions of DACS are modified  
such that 7-aminocephems or 7-aminocephams (including 3-  
exomethylenecephams) or other bicyclic  $\beta$ -lactams may be produced *in vitro*  
20 or *in vivo* from 6-amino penicillins (such as 6-aminopenicillanic acid) or  
cephams or cephems (Scheme 17). The process may include the  
following modifications:

25 R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S  
30 S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y

A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C  
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y.  
5 R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I  
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L  
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S  
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

10 It is recognised that these modifications may have to be  
made in conjunction with each other or with other modifications in order to  
produce a useful catalyst with the desired properties. Other modifications  
based on the use of the three dimensional structure of IPNS, DACS,  
DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of  
15 these enzymes to their substrates, intermediates, modifiers, products or  
inhibitors are not excluded.

n) The side chain binding interactions of DACS are modified  
such that cephams or cephalosporins without any substituent at the 7-  
20 position or other bicyclic  $\beta$ -lactams, without any substituent at the 7-position,  
may be produced *in vitro* or *in vivo* from penicillins or cepham substrates,  
such as penicillanic acid (Scheme 18). The penicillanic acid may be  
produced whether *in vitro* or *in vivo*. The process may include the following  
modifications:

25 R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
30 C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S

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S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
5 T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C  
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I  
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L  
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S  
10 R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

20 o) DACS is modified to produce 3-exomethylenecephams with hydrophobic side chains (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor.) (Scheme 19). The process will involve modification of both the side chain binding interactions of DACS substrates and of the thiaxolidine or cepham binding interactions and may 25 involve the use of penicillins with hydrophobic side chains (e.g. penicillin G or V) as substrates or the use of other unnatural substrates. The process may include the following modifications:

30 V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

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L223F/A/G/V//I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P  
T221F/A/G/V//I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
M211A/G/V//I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F  
5 L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V  
P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/V  
R279F/A/G/V//I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y  
S281F/A/G/V//I/L/W/M/N/C/N/P/T/E/D/R/K/H/Q/Y  
N230F/A/G/V//I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y  
10 Q225F/A/G/V//I/L/W/M/N/C/N/P/S/T/E/D/R/K/H/Y  
F252F/A/G/V//I/L/W/M/N/C/P/S/T/E/D/R/K/H/Q/Y  
R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
15 F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S  
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
20 P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C  
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I  
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L  
25 R210F/A/G/V//I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be  
made in conjunction with each other or with other modifications in order to  
produce a useful catalyst with the desired properties. Other modifications  
30 based on the use of the three dimensional structure of IPNS, DACS,

DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

5 p) The structure of DAOCS/DACS is modified in its active site region to accept natural or unnatural substrates (including, but not exclusively, penicillin N, adipoyl penicillin) to produce bicyclic  $\beta$ -lactams other than cephalosporins of commercial use (Scheme 20). For example the region of DAOCS/DACS interacting with the thiazolidine ring of its  
10 natural substrate penicillin N (or the cepham ring of DAOC) may be modified such that the modified DAOCS/DACS produces 3-exomethylenecephams from penicillin N, penicillin G, or penicillin V, or other substrates for DAOCS/DACS. The process may include the following modifications:

15

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P  
20 T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
M211A/G/V/I/L/T/W/C/N/P/S/E/D/R/K/H/Q/Y/F  
L187F/A/G/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V  
P185F/A/G/I/L/T/W/M/C/N/S/E/D/R/K/H/Q/Y/V  
L189A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/F  
25 R279F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/K/H/Q/Y  
S281F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y  
N230F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y  
Q225F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Y  
F252F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y  
30 R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

- 29 -

R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications 5 based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

10 q) The side chain binding interactions of DAOCS/DACS are modified such that 7-aminocephems or 7-aminocephams (including 3-exomethylenecephams) or other bicyclic  $\beta$ -lactams may be produced *in vitro* or *in vivo* from 6-amino penicillins (e.g. 6-aminopenicillanic acid) or cephams or cephems (Scheme 21). The process may include the 15 following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

20 L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R

C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S

S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y

F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y

A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q

25 P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y

T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y

T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y

M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y

L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

30 R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I

- 30 -

Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q

R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

5 It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of 10 these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

15 r) The side chain binding interactions of DAOCS/DACS are modified such that cephams or cephalosporins without any substituent at the 7-position or other bicyclic  $\beta$ -lactams, without any substituent at the 7-position, may be produced *in vitro* or *in vivo* from penicillins or cepham substrates, such as penicillanic acid. The penicillanic acid may be produced whether *in vitro* or *in vivo* (Scheme 22). The process may include the following modifications:

20 R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R  
25 C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S  
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
30 T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y

T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y  
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I  
5 Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q  
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S  
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

it is recognised that these modifications may have to be  
10 made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or  
15 inhibitors are not excluded.

s) DAOCS/DACS is modified to produce 3-exomethylenecephams with hydrophobic side chains (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor) (Scheme 23). The process will involve modification of both the side chain binding interactions of DAOCS/DACS substrates and of the thiaxolidine or cepham binding interactions and may involve the use of penicillins with hydrophobic side chains (e.g. penicillin G or V) as substrates or the use of other unnatural substrates. The process may  
20 include the following modifications:  
25

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
30 L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R

S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
5 T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y  
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I  
10 Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q  
V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P  
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
15 M211A/G/V/I/L/T/W/C/N/P/S/E/D/R/K/H/Q/Y/F  
L187F/A/G/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V  
P185F/A/G/I/L/T/W/M/C/N/S/E/D/R/K/H/Q/Y/V  
F189A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
R279F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/K/H/Q/Y  
20 S281F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y  
N230F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y  
Q225F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Y  
F252F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y  
25 R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S  
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be  
made in conjunction with each other or with other modifications in order to  
30 produce a useful catalyst with the desired properties. Other modifications

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produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or 5 inhibitors are not excluded.

10 t) The structure of DAOC/DACS is modified in its active site region to accept substrates (i.e. penicillins with hydrophobic side chains, (including, but not exclusively, penicillin N, penicillin G and penicillin V) to produce cephalosporins or other bicyclic  $\beta$ -lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 24). The process 15 may include the following modifications:

15 R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y  
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R  
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S  
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y  
20 F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y  
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q  
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y  
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
T217F/A/G/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y  
25 M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y  
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y  
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I  
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q  
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S  
30 R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, 5 DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

Use can also be made of the 3D structure of IPNS to determine or predict the structure of other related enzymes which are not active in the penicillin or cephalosporin biosynthesis pathway. The 10 structural information so obtained can then be used to modify the other enzyme or for designing an inhibitor for the other enzymes. Such other enzymes include flavone synthase, prolyl hydroxylase, proline hydroxylase, lysyl hydroxylase, aspartyl hydroxylase, flavanone 3 $\beta$ -hydroxylase, 15 gibberellin C-20 oxidase, gibberellin 3 $\beta$ -hydroxylase, *para*-hydroxyphenylpyruvate dioxygenase (HPPD), 1-aminocyclopropane-1-carboxylic acid (ACC) oxidase. Specific embodiments envisaged include:

- The modification of the oxidases involved in gibberellin biosynthesis in order that modified enzymes may be introduced into plants 20 in order to improve crop production.
- The design of inhibitors of ACC oxidase to be used for the control of fruit ripening.
- The design and use of inhibitors of prolyl hydroxylase for use in the treatment of arthritis and related diseases.

25 Modification of enzymes may conveniently be effected at the nucleic acid stage. Thus, the present invention envisages genes which code for the modified enzymes herein described. The nucleic acid sequence of such genes may be readily predicted. Mutations of existing wild-type genes may readily be effected e.g. by the use of commercially 30 available mutagenesis kits.

The gene may be introduced into an expression vector by techniques which are well known. The expression vector may be used to transform a host micro-organism, such as for example *Penicillium chrysogenum* or *Acremonium chrysogenum*, again by techniques which are well known. The micro-organism should be capable of expressing the gene under fermentation conditions, e.g. by having the gene under the transcriptional and translational regulation of fungal expression signals. Such micro-organisms containing the modified gene may be used to make bicyclic  $\beta$ -lactams of the penicillin or cephalosporin family, again by techniques which are well known.

10 The following experiments were performed to demonstrate the invention.

#### EXAMPLE 1

15 A U.S.E mutagenesis kit (Pharmacia) was used for all the mutagenesis reactions and a *Pst* I restriction site on the pET vector was selected. Selection of single and double mutants were successfully performed from colonies by restriction enzyme digestion. (Sambrook et al, Molecular Cloning, A Laboratory Manual, Cold Spring Harbour, USA, 1989). It was found that about 50% of colonies selected were mutants.

20 Mutations of DAOCS (Table 1) were confirmed by sequencing according to the dideoxy method of Sanger. Mutants were designed after study of the IPNS- $Mn^{2+}$  and the IPNS-Fe(II)-ACV structures. Polar residues with which the side chain D- $\alpha$ -amino adipoyl (carboxylate and amino groups) might bind to were identified.

25 Almost all the mutants expressed well, except R88I, R88Q and R87Q/R287Q whereby the expression level was only about half of others. Generally the expression level of colonies was about 10~20 % of soluble protein at 27°C. Moreover, recombinant enzyme of P168V mutant 30 was insoluble. These mutant enzymes were purified to ~60-70 % purity

with Resource-Q column (Pharmacia). The activity of each mutant with respect to penicillin N and its side-chain analogues was analysed by bioassay. It was found that R87I, R87Q, R88I and R88Q could inhibit the growth of *E coli* X580 cells using a hole-plate assay which contained 5 penicillinase. The products of the reaction with penicillin G and wild type DAOCS also showed the same inhibition. Screening of the substrate conversion of penicillins mutants was also performed using a assay with radiolabelled  $\alpha$ -ketoglutarate. The reaction conditions were the same as for bioassay except that [ $^{14}\text{C}$ ]- $\alpha$ -ketoglutarate was used. The specific 10 activities of the various mutants are summarised in Table I.

The loss of activity when using penicillin N as a substrate after mutation of arginine 287 to isoleucine or glutamine in the active site of expandase implies an important interaction of this amino acid with the carboxyl group which located in the side chain of penicillin N. This is 15 compatible with the structural predictions for DAOCS which were suggested based on IPNS structure. On the other hand, mutation at arginine 87 to isoleucine or glutamine enhanced the activity (when using penicillin N as a substrate), whereas mutants of arginine 88 caused partial 20 loss of activity (when using penicillin N as a substrate). Double mutations at the sites totally eliminated activity.

The specific activities of the (mutant) modified DAOCS, when using penicillin N as a substrate, support the prediction that the 3-dimensional structure of DAOCS is closely related to that of IPNS. However, not all the kinetic results can be predicted by analysis of the 25 predicted DAOC structure, e.g. the apparent increase in activity of the R87Q modification, when using penicillin N as a substrate. Other results in Table 1 further demonstrate the invention. For example the R87Q mutant converts penicillin G to phenylacetylcephalosporin G more efficiently than the unmodified enzyme. Other results demonstrate the introduction of new 30 activities into the modified DAOCS enzymes. For example neither oxacillin

nor piperacillin are substrates for the unmodified enzymes, but are substrates for the R87I/R287Q modified enzymes.

## EXAMPLE 2

### 5 IPNS-Fe-ACV Complex

#### **Enzyme and Substrate Preparation**

Recombinant *A. nidulans* IPNS was purified as the apo-enzyme as described previously (Roach *et al*, Protein Science, 1995, 4, 1007-1009) and stored at -80°C in 75µl aliquots (50 mg/ml in 20 mM Tris-10 HCl, pH 8.0). ACV (thiol form) was prepared as described previously and was further purified by HPLC [Hypersil octadecylsilane (C<sub>18</sub>) column (250 x 10 mm), eluting with 10 mM NH<sub>4</sub>CO<sub>3</sub>, containing 4% (vol./vol.) MeOH; R<sub>t</sub>=6.5 min at 4 ml/min], freeze dried and stored as 2 mg aliquots.

### 15 **Crystallisation**

Crystallisation trials were performed at 17°C under anaerobic conditions (<0.2 ppm O<sub>2</sub>) in a glove box (Belle Technology, Portesham, Dorset, UK) using the hanging drop vapour diffusion technique. All solutions except the protein were deoxygenated by repeated evacuation followed by argon flushing (repeated three times) prior to transfer to the anaerobic glove box. Solid reagents (ACV, ferrous sulphate and sodium dithionite), all solutions except protein solutions, washed cover-slips and greased Linbro plates were left for 16 h in the glove box to further deoxygenate. IPNS solutions were transferred to the glove box immediately prior to each crystallisation experiment and mixed by repeated gentle pipetting to assist deoxygenation. To further ensure that the crystallisation experiments were done anaerobically, a coloured redox indicator was added to each well. Thus, oxidised resazurin which shows a mauve to colourless change upon dithionite reduction, was added (0.001% mass/vol.) to the stock well solutions (separate solutions, without

resazurin, were reserved for hanging drops) and sodium dithionite solution (100 mM) added dropwise until the solution in the well changed colour from mauve to colourless (Jacob, Methods in Microbiol., 1969, **2**, 91-124). Upon exposure to oxygen (either by contamination or upon withdrawing the 5 crystallisation tray from the glove box), the solution in the well changed from colourless (reduced) to pink (partially oxidised).

A stock solution containing ferrous sulphate (5 mM), ACV (80 mM) and IPNS (50 mg/ml, 1.35 mM) was then prepared and used in random screening experiments using 6  $\mu$ l drops (1:1 precipitant:protein) 10 (Jancerik and Kim, J. Appl. Crystallogr., 1991, **24**, 409). Three crystal forms were obtained using a precipitant solution containing 1.8M lithium sulphate and 100 mM Tris-HCl (pH 8.5). Crystals were not observed in analogous crystallisation experiments carried out in the absence of ACV. Crystallisation conditions were optimised by varying the protein and 15 precipitant concentrations.

Plate crystals (Form I) typically appeared between 6 and 12 hours and reached a maximum size (typically  $500 \times 150 \times 25 \mu\text{m}^3$ ) in 48 hours. Hexagonal columnar crystals (Form II) typically appeared after 12 - 16 hours and grew to a maximum size (typically  $1000 \times 500 \times 500 \mu\text{m}^3$ ) in 1 20 week. The needles (Form III), with a hexagonal cross-section, appeared after ca. 2 weeks and were more commonly observed when using less homogenous batches of protein. In analogous experiments carried out under aerobic conditions, no crystals were observed.

Form I crystals grew spontaneously in less than half of the 25 drops after 12 hours. After this time, Form II crystals began to grow and predominated in those drops in which plates had not grown. By using serial dilutions of microseeds prepared from either Form I or Form II crystals, it was possible to bias the growth of crystals completely to either 30 of these morphologies. There is a delicate balance between production of the different forms since some drops contained two or all three of the

different crystal forms.

### X-ray Analysis

For initial characterisation, crystals were mounted in quartz capillaries under an anaerobic atmosphere and the capillaries sealed with wax. Data were then collected (Table 4) at room temperature. Subsequently, the crystals were shown to be apparently stable to relatively short (< 1 hour) exposure to oxygen and were withdrawn from the glove box. The crystals were then rapidly transferred to a cryoprotective mother liquor (100 mM Tris-HCl pH 8.5, 20% (vol./vol.) glycerol, saturated at room temperature with lithium sulphate) and frozen using a Cryostream (Oxford Cryosystems). Data were then collected at 100 K. Data were analysed using the programs DENZO and SCALEPACK (Otinowski, Data Collection and Processing, Daresbury Laboratory, Warrington, UK (Sawyer et al, Eds) PL/SCI/R34, pp 55-62).

**Table 4 - Crystal Statistics**

| Crysta<br>l Form | Diffractio<br>n Limit<br>(nm)† | Space<br>Group                                | Unit Cell<br>Dimensions<br>(nm) | Solvent<br>Content<br>(%) | Completeness<br>(%) | Rsym<br>(%) |
|------------------|--------------------------------|---|---------------------------------|---------------------------|---------------------|-------------|
| I                | 0.11, 0.18                     | P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> | 4.68, 7.15, 10.10               | 38.5                      | 95.4                | 5.9         |
| II               | 0.21, 0.23                     | P3 <sub>1</sub> 2 <sub>1</sub>                | 10.10, 10.10,<br>11.567         | 69.5                      | 94.0                | 7.2         |

† The first figure refers to the diffraction limit of the form I and form II crystals after respectively 30 and 10s exposures at BL19 of the European Synchrotron Radiation Facility (ESRF). The second figure refers to the diffraction limits after 30 min. exposures using a Rikagu rotating anode source operating at 60 kV and 70 mA equipped with a MAR Research

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imaging plate detector. All other figures in the table refer to data collected at the ESRF. The data for form I crystals was collected using a MAR Research imaging plate detector and the data for the form II crystals on a charged coupled device detector.

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Hereafter:

Table 1 appears on page 41.

Table 2 appears on pages 42-78.

Table 3 appears on pages 79-119.

Reaction Schemes on pages 120-129.

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Table 1: The Specific activity of various DAOCS mutants analysed by the turnover of  $\alpha$ -[ $^{14}\text{C}$ ]-ketoglutarate.

| Specific activity (nmol/min/mg) | Penicillin N | 6-Amino-penicillanic acid (6-APA) | Adipyl-6-APA | Penicillin G | Penicillin V | Ampicillin | Carbenicillin | Ammoxicillin | Methicillin | Cloxacillin | Oxacillin | Piperacillin |
|---------------------------------|--------------|-----------------------------------|--------------|--------------|--------------|------------|---------------|--------------|-------------|-------------|-----------|--------------|
| 6.4±0.5*                        | 1.0±0.2      | 2.7±0.4                           | 5.1±0.4      | 5.3±0.3      | 0            | 0          | 1.4±0.6       | 0            | 1.6±0.6     | 0           | 0         | 1.8±0.2      |
| Wild type                       | 0            | 1.7±0.6                           | 0            | 0            | 2.3±0.2      | 0          | 0             | 1.1±0.04     | 0.2±0.1     | 2.7±0.6     | 2.0±0.09  | 0            |
| R287I                           | 0            | 0                                 | 0            | 0            | 0            | 0          | 0             | 0            | 0           | 0           | 0         | 0            |
| R287Q                           | 0            | 0                                 | 0            | 4.3±0.1      | 1.5±0.3      | 0          | 0             | 0            | 0           | 0.9±0.04    | 0.8±0.3   | 0            |
| R87I                            | 6.4±0.05     | 1.1±0.5                           | 0            | 7.5±0.4      | 3.4±0.6      | 0          | 0             | 0            | 0           | 0           | 0         | 0            |
| R87Q                            | 13.4±0.4     | 0                                 | 0            | 2.5±0.5      | 0            | 0          | 0             | 0            | 0           | 0           | 0         | 0            |
| R88I                            | 5.3±0.8      | 0                                 | 0            | 0.2±0.02     | 0            | 0          | 0             | 0            | 0           | 0           | 0         | 0            |
| R88Q                            | 2.9±0.5      | 0                                 | 0            | 0.03±0.04    | 0            | 0          | 0             | 0            | 0           | 0           | 0         | 0            |
| R87I/R287I                      | 0            | 0                                 | 0            | 0            | 0            | 0          | 0             | 0            | 0           | 0           | 0         | 0            |
| R87Q/R287I                      | 0            | 0                                 | 0            | 0            | 0            | 0          | 0             | 1.1±0.3      | 0           | 4.5±0.08    | 4.1±0.4   | 2.5±0.3      |
| R87I/R287Q                      | 0            | 3.3±0.2                           | 0            | 3.2±0.1      | 0.7±0.2      | 0          | 0             | 0            | 0           | 0           | 0         | 0            |
| R87Q/R287Q                      | 0            | 0                                 | 0            | 0            | 0            | 0          | 0             | 0            | 0           | 0           | 0         | 0            |

\* Experiments were done in duplicate and values for "the penicillin uncoupled decarboxylation of  $\alpha$ -ketoglutarate" have been subtracted.

The specific radioactivity of the  $\alpha$ -ketoglutarate used was ca. 0.057  $\mu\text{Ci}/\mu\text{mol}$ .

N.B. "The penicillin uncoupled decarboxylation reaction" is the enzymatic turnover of  $\alpha$ -ketoglutarate in the absence of penicillin substrate.

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Table 2

|        |          |          |          |       |         |        |         |      |
|--------|----------|----------|----------|-------|---------|--------|---------|------|
| CRYST1 | 59.200   | 127.000  | 139.600  | 90.00 | 90.00   | 90.00  |         |      |
| SCALE1 | 0.016892 | 0.000000 | 0.000000 |       |         |        | 0.00000 |      |
| SCALE2 | 0.000000 | 0.007874 | 0.000000 |       |         |        | 0.00000 |      |
| SCALE3 | 0.000000 | 0.000000 | 0.007163 |       |         |        | 0.00000 |      |
| ATOM   | 1        | CB       | VAL A    | 4     | 16.524  | 53.636 | -2.826  |      |
| ATOM   | 2        | CG1      | VAL A    | 4     | 15.692  | 54.759 | -2.223  | 1.00 |
| ATOM   | 3        | CG2      | VAL A    | 4     | 18.011  | 53.869 | -2.523  | 1.00 |
| ATOM   | 4        | C        | VAL A    | 4     | 14.636  | 52.001 | -2.797  | 1.00 |
| ATOM   | 5        | O        | VAL A    | 4     | 14.443  | 51.769 | -3.987  | 1.00 |
| ATOM   | 6        | N        | VAL A    | 4     | 16.880  | 51.117 | -2.818  | 1.00 |
| ATOM   | 7        | CA       | VAL A    | 4     | 16.049  | 52.254 | -2.290  | 1.00 |
| ATOM   | 8        | N        | SER A    | 5     | 13.655  | 52.015 | -1.916  | 1.00 |
| ATOM   | 9        | CA       | SER A    | 5     | 12.286  | 51.764 | -2.350  | 1.00 |
| ATOM   | 10       | CB       | SER A    | 5     | 11.583  | 50.804 | -1.380  | 1.00 |
| ATOM   | 11       | OG       | SER A    | 5     | 12.012  | 51.018 | -0.044  | 1.00 |
| ATOM   | 12       | C        | SER A    | 5     | 11.474  | 53.054 | -2.482  | 1.00 |
| ATOM   | 13       | O        | SER A    | 5     | 11.970  | 54.146 | -2.187  | 1.00 |
| ATOM   | 14       | N        | LYS A    | 6     | 10.250  | 52.914 | -2.970  | 1.00 |
| ATOM   | 15       | CA       | LYS A    | 6     | 9.320   | 54.025 | -3.124  | 1.00 |
| ATOM   | 16       | CB       | LYS A    | 6     | 8.403   | 53.799 | -4.319  | 1.00 |
| ATOM   | 17       | CG       | LYS A    | 6     | 8.751   | 54.568 | -5.557  | 1.00 |
| ATOM   | 18       | CD       | LYS A    | 6     | 7.579   | 54.445 | -6.510  | 1.00 |
| ATOM   | 19       | CE       | LYS A    | 6     | 7.768   | 55.261 | -7.784  | 1.00 |
| ATOM   | 20       | NZ       | LYS A    | 6     | 6.509   | 55.312 | -8.612  | 1.00 |
| ATOM   | 21       | C        | LYS A    | 6     | 8.457   | 54.095 | -1.868  | 1.00 |
| ATOM   | 22       | O        | LYS A    | 6     | 8.061   | 53.061 | -1.325  | 1.00 |
| ATOM   | 23       | N        | ALA A    | 7     | 8.166   | 55.304 | -1.410  | 1.00 |
| ATOM   | 24       | CA       | ALA A    | 7     | 7.346   | 55.487 | -0.231  | 1.00 |
| ATOM   | 25       | CB       | ALA A    | 7     | 7.632   | 56.632 | 0.393   | 1.00 |
| ATOM   | 26       | C        | ALA A    | 7     | 5.875   | 55.363 | -0.609  | 1.00 |
| ATOM   | 27       | O        | ALA A    | 7     | 5.469   | 55.706 | -1.721  | 1.00 |
| ATOM   | 28       | N        | ASN A    | 8     | 5.080   | 54.840 | 0.313   | 1.00 |
| ATOM   | 29       | CA       | ASN A    | 8     | 3.652   | 54.694 | 0.086   | 1.00 |
| ATOM   | 30       | CB       | ASN A    | 8     | 3.041   | 53.759 | 1.142   | 1.00 |
| ATOM   | 31       | CG       | ASN A    | 8     | 1.515   | 53.798 | 1.154   | 1.00 |
| ATOM   | 32       | OD1      | ASN A    | 8     | 0.865   | 53.318 | 0.226   | 1.00 |
| ATOM   | 33       | ND2      | ASN A    | 8     | 0.941   | 54.403 | 2.193   | 1.00 |
| ATOM   | 34       | C        | ASN A    | 8     | 3.009   | 56.078 | 0.175   | 1.00 |
| ATOM   | 35       | O        | ASN A    | 8     | 2.782   | 56.594 | 1.276   | 1.00 |
| ATOM   | 36       | N        | VAL A    | 9     | 2.802   | 56.712 | -0.977  | 1.00 |
| ATOM   | 37       | CA       | VAL A    | 9     | 2.167   | 58.028 | -1.026  | 1.00 |
| ATOM   | 38       | CB       | VAL A    | 9     | 3.066   | 59.093 | -1.733  | 1.00 |
| ATOM   | 39       | CG1      | VAL A    | 9     | 2.425   | 60.459 | -1.650  | 1.00 |
| ATOM   | 40       | CG2      | VAL A    | 9     | 4.438   | 59.149 | -1.100  | 1.00 |
| ATOM   | 41       | C        | VAL A    | 9     | 0.835   | 57.869 | -1.768  | 1.00 |
| ATOM   | 42       | O        | VAL A    | 9     | 0.785   | 57.827 | -3.000  | 1.00 |
| ATOM   | 43       | N        | PRO A    | 10    | -0.261  | 57.715 | -1.018  | 1.00 |
| ATOM   | 44       | CD       | PRO A    | 10    | -0.322  | 57.622 | 0.451   | 1.00 |
| ATOM   | 45       | CA       | PRO A    | 10    | -1.588  | 57.549 | -1.620  | 1.00 |
| ATOM   | 46       | CB       | PRO A    | 10    | -2.473  | 57.229 | -0.412  | 1.00 |
| ATOM   | 47       | CG       | PRO A    | 10    | -1.775  | 57.912 | 0.734   | 1.00 |
| ATOM   | 48       | C        | PRO A    | 10    | -2.094  | 58.759 | -2.390  | 1.00 |
| ATOM   | 49       | O        | PRO A    | 10    | -1.778  | 59.897 | -2.060  | 1.00 |
| ATOM   | 50       | N        | LYS A    | 11    | -2.870  | 58.503 | -3.434  | 1.00 |
| ATOM   | 51       | CA       | LYS A    | 11    | -3.435  | 59.576 | -4.236  | 1.00 |
| ATOM   | 52       | CB       | LYS A    | 11    | -3.361  | 59.233 | -5.724  | 1.00 |
| ATOM   | 53       | CG       | LYS A    | 11    | -1.958  | 58.944 | -6.203  | 1.00 |
| ATOM   | 54       | CD       | LYS A    | 11    | -1.858  | 58.929 | -7.722  | 1.00 |
| ATOM   | 55       | CE       | LYS A    | 11    | -0.482  | 58.455 | -8.166  | 1.00 |
| ATOM   | 56       | NZ       | LYS A    | 11    | 0.620   | 59.309 | -7.628  | 1.00 |
| ATOM   | 57       | C        | LYS A    | 11    | -4.882  | 59.740 | -3.798  | 1.00 |
| ATOM   | 58       | O        | LYS A    | 11    | -5.748  | 58.984 | -4.232  | 1.00 |
| ATOM   | 59       | N        | ILE A    | 12    | -5.133  | 60.704 | -2.917  | 1.00 |
| ATOM   | 60       | CA       | ILE A    | 12    | -6.474  | 60.959 | -2.394  | 1.00 |
| ATOM   | 61       | CB       | ILE A    | 12    | -6.407  | 61.510 | -0.965  | 1.00 |
| ATOM   | 62       | CG2      | ILE A    | 12    | -7.803  | 61.826 | -0.436  | 1.00 |
| ATOM   | 63       | CG1      | ILE A    | 12    | -5.682  | 60.505 | -0.077  | 1.00 |
| ATOM   | 64       | CD1      | ILE A    | 12    | -5.414  | 60.995 | 1.314   | 1.00 |
| ATOM   | 65       | C        | ILE A    | 12    | -7.268  | 61.932 | -3.250  | 1.00 |
| ATOM   | 66       | O        | ILE A    | 12    | -6.729  | 62.919 | -3.749  | 1.00 |
| ATOM   | 67       | N        | ASP A    | 13    | -8.544  | 61.622 | -3.451  | 1.00 |
| ATOM   | 68       | CA       | ASP A    | 13    | -9.431  | 62.484 | -4.225  | 1.00 |
| ATOM   | 69       | CB       | ASP A    | 13    | -10.555 | 61.684 | -4.881  | 1.00 |

51.16

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|      |     |     |       |    |         |        |        |      |       |
|------|-----|-----|-------|----|---------|--------|--------|------|-------|
| ATOM | 70  | CG  | ASP A | 13 | -11.361 | 62.512 | -5.869 | 1.00 | 56.62 |
| ATOM | 71  | OD1 | ASP A | 13 | -11.737 | 63.659 | -5.544 | 1.00 | 54.34 |
| ATOM | 72  | OD2 | ASP A | 13 | -11.619 | 62.011 | -6.984 | 1.00 | 66.60 |
| ATOM | 73  | C   | ASP A | 13 | -10.000 | 63.472 | -3.227 | 1.00 | 44.39 |
| ATOM | 74  | O   | ASP A | 13 | -10.791 | 63.121 | -2.354 | 1.00 | 44.73 |
| ATOM | 75  | N   | VAL A | 14 | -9.605  | 64.719 | -3.391 | 1.00 | 44.33 |
| ATOM | 76  | CA  | VAL A | 14 | -10.003 | 65.785 | -2.498 | 1.00 | 38.69 |
| ATOM | 77  | CB  | VAL A | 14 | -8.796  | 66.720 | -2.338 | 1.00 | 34.66 |
| ATOM | 78  | CG1 | VAL A | 14 | -9.190  | 68.101 | -1.875 | 1.00 | 37.77 |
| ATOM | 79  | CG2 | VAL A | 14 | -7.833  | 66.077 | -1.365 | 1.00 | 33.42 |
| ATOM | 80  | C   | VAL A | 14 | -11.296 | 66.521 | -2.846 | 1.00 | 39.30 |
| ATOM | 81  | O   | VAL A | 14 | -11.808 | 67.298 | -2.036 | 1.00 | 39.59 |
| ATOM | 82  | N   | SER A | 15 | -11.891 | 66.202 | -3.990 | 1.00 | 38.33 |
| ATOM | 83  | CA  | SER A | 15 | -13.116 | 66.881 | -4.393 | 1.00 | 37.64 |
| ATOM | 84  | CB  | SER A | 15 | -13.686 | 66.298 | -5.689 | 1.00 | 39.61 |
| ATOM | 85  | OG  | SER A | 15 | -14.027 | 64.933 | -5.546 | 1.00 | 47.59 |
| ATOM | 86  | C   | SER A | 15 | -14.197 | 66.977 | -3.324 | 1.00 | 37.35 |
| ATOM | 87  | O   | SER A | 15 | -14.691 | 68.066 | -3.056 | 1.00 | 40.20 |
| ATOM | 88  | N   | PRO A | 16 | -14.532 | 65.866 | -2.647 | 1.00 | 38.58 |
| ATOM | 89  | CD  | PRO A | 16 | -13.957 | 64.511 | -2.714 | 1.00 | 40.22 |
| ATOM | 90  | CA  | PRO A | 16 | -15.574 | 65.918 | -1.613 | 1.00 | 37.63 |
| ATOM | 91  | CB  | PRO A | 16 | -15.410 | 64.583 | -0.901 | 1.00 | 33.25 |
| ATOM | 92  | CG  | PRO A | 16 | -14.999 | 63.689 | -1.991 | 1.00 | 36.58 |
| ATOM | 93  | C   | PRO A | 16 | -15.439 | 67.066 | -0.624 | 1.00 | 38.86 |
| ATOM | 94  | O   | PRO A | 16 | -16.442 | 67.614 | -0.184 | 1.00 | 40.71 |
| ATOM | 95  | N   | LEU A | 17 | -14.200 | 67.444 | -0.310 | 1.00 | 39.30 |
| ATOM | 96  | CA  | LEU A | 17 | -13.917 | 68.513 | 0.649  | 1.00 | 38.18 |
| ATOM | 97  | CB  | LEU A | 17 | -12.412 | 68.594 | 0.911  | 1.00 | 34.24 |
| ATOM | 98  | CG  | LEU A | 17 | -11.838 | 67.299 | 1.490  | 1.00 | 32.70 |
| ATOM | 99  | CD1 | LEU A | 17 | -10.330 | 67.382 | 1.663  | 1.00 | 27.81 |
| ATOM | 100 | CD2 | LEU A | 17 | -12.515 | 67.008 | 2.820  | 1.00 | 34.84 |
| ATOM | 101 | C   | LEU A | 17 | -14.472 | 69.881 | 0.260  | 1.00 | 41.67 |
| ATOM | 102 | O   | LEU A | 17 | -14.598 | 70.776 | 1.105  | 1.00 | 38.36 |
| ATOM | 103 | N   | PHE A | 18 | -14.774 | 70.043 | -1.025 | 1.00 | 48.11 |
| ATOM | 104 | CA  | PHE A | 18 | -15.339 | 71.287 | -1.551 | 1.00 | 52.21 |
| ATOM | 105 | CB  | PHE A | 18 | -14.857 | 71.551 | -2.993 | 1.00 | 51.38 |
| ATOM | 106 | CG  | PHE A | 18 | -13.365 | 71.738 | -3.132 | 1.00 | 49.52 |
| ATOM | 107 | CD1 | PHE A | 18 | -12.552 | 70.679 | -3.513 | 1.00 | 50.16 |
| ATOM | 108 | CD2 | PHE A | 18 | -12.781 | 72.983 | -2.932 | 1.00 | 47.59 |
| ATOM | 109 | CE1 | PHE A | 18 | -11.183 | 70.857 | -3.695 | 1.00 | 50.47 |
| ATOM | 110 | CE2 | PHE A | 18 | -11.413 | 73.166 | -3.114 | 1.00 | 44.37 |
| ATOM | 111 | CZ  | PHE A | 18 | -10.616 | 72.102 | -3.496 | 1.00 | 45.21 |
| ATOM | 112 | C   | PHE A | 18 | -16.871 | 71.202 | -1.550 | 1.00 | 53.42 |
| ATOM | 113 | O   | PHE A | 18 | -17.550 | 72.180 | -1.848 | 1.00 | 53.80 |
| ATOM | 114 | N   | GLY A | 19 | -17.407 | 70.020 | -1.259 | 1.00 | 56.82 |
| ATOM | 115 | CA  | GLY A | 19 | -18.847 | 69.842 | -1.247 | 1.00 | 60.49 |
| ATOM | 116 | C   | GLY A | 19 | -19.502 | 69.931 | 0.120  | 1.00 | 64.67 |
| ATOM | 117 | O   | GLY A | 19 | -18.927 | 70.470 | 1.071  | 1.00 | 64.98 |
| ATOM | 118 | N   | ASP A | 20 | -20.738 | 69.441 | 0.200  | 1.00 | 69.36 |
| ATOM | 119 | CA  | ASP A | 20 | -21.507 | 69.443 | 1.449  | 1.00 | 72.36 |
| ATOM | 120 | CB  | ASP A | 20 | -22.799 | 70.263 | 1.310  | 1.00 | 76.50 |
| ATOM | 121 | CG  | ASP A | 20 | -22.543 | 71.760 | 1.234  | 1.00 | 83.77 |
| ATOM | 122 | OD1 | ASP A | 20 | -21.889 | 72.300 | 2.152  | 1.00 | 89.42 |
| ATOM | 123 | OD2 | ASP A | 20 | -23.002 | 72.400 | 0.262  | 1.00 | 85.64 |
| ATOM | 124 | C   | ASP A | 20 | -21.861 | 68.035 | 1.918  | 1.00 | 70.68 |
| ATOM | 125 | O   | ASP A | 20 | -22.433 | 67.865 | 2.992  | 1.00 | 71.00 |
| ATOM | 126 | N   | ASP A | 21 | -21.533 | 67.030 | 1.111  | 1.00 | 68.45 |
| ATOM | 127 | CA  | ASP A | 21 | -21.830 | 65.653 | 1.473  | 1.00 | 66.91 |
| ATOM | 128 | CB  | ASP A | 21 | -21.643 | 64.720 | 0.267  | 1.00 | 69.88 |
| ATOM | 129 | CG  | ASP A | 21 | -22.015 | 63.268 | 0.574  | 1.00 | 73.83 |
| ATOM | 130 | OD1 | ASP A | 21 | -22.477 | 62.978 | 1.702  | 1.00 | 76.66 |
| ATOM | 131 | OD2 | ASP A | 21 | -21.845 | 62.409 | -0.322 | 1.00 | 76.24 |
| ATOM | 132 | C   | ASP A | 21 | -20.917 | 65.240 | 2.625  | 1.00 | 65.51 |
| ATOM | 133 | O   | ASP A | 21 | -19.785 | 64.800 | 2.419  | 1.00 | 67.20 |
| ATOM | 134 | N   | GLN A | 22 | -21.433 | 65.365 | 3.838  | 1.00 | 63.04 |
| ATOM | 135 | CA  | GLN A | 22 | -20.687 | 65.018 | 5.033  | 1.00 | 59.99 |
| ATOM | 136 | CB  | GLN A | 22 | -21.578 | 65.138 | 6.264  | 1.00 | 60.92 |
| ATOM | 137 | CG  | GLN A | 22 | -20.821 | 65.550 | 7.505  | 1.00 | 68.34 |
| ATOM | 138 | CD  | GLN A | 22 | -20.120 | 66.894 | 7.326  | 1.00 | 74.81 |
| ATOM | 139 | OE1 | GLN A | 22 | -20.632 | 67.793 | 6.649  | 1.00 | 78.00 |
| ATOM | 140 | NE2 | GLN A | 22 | -18.931 | 67.028 | 7.909  | 1.00 | 77.30 |
| ATOM | 141 | C   | GLN A | 22 | -20.104 | 63.623 | 4.971  | 1.00 | 58.00 |
| ATOM | 142 | O   | GLN A | 22 | -18.965 | 63.402 | 5.384  | 1.00 | 59.37 |

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|      |     |     |       |    |         |        |        |      |       |
|------|-----|-----|-------|----|---------|--------|--------|------|-------|
| ATOM | 143 | N   | ALA A | 23 | -20.877 | 62.688 | 4.428  | 1.00 | 55.74 |
| ATOM | 144 | CA  | ALA A | 23 | -20.448 | 61.294 | 4.323  | 1.00 | 57.85 |
| ATOM | 145 | CB  | ALA A | 23 | -21.550 | 60.444 | 3.688  | 1.00 | 57.01 |
| ATOM | 146 | C   | ALA A | 23 | -19.142 | 61.133 | 3.547  | 1.00 | 58.62 |
| ATOM | 147 | O   | ALA A | 23 | -18.180 | 60.534 | 4.040  | 1.00 | 59.15 |
| ATOM | 148 | N   | ALA A | 24 | -19.112 | 61.662 | 2.329  | 1.00 | 57.88 |
| ATOM | 149 | CA  | ALA A | 24 | -17.920 | 61.567 | 1.505  | 1.00 | 54.77 |
| ATOM | 150 | CB  | ALA A | 24 | -18.195 | 62.086 | 0.097  | 1.00 | 52.07 |
| ATOM | 151 | C   | ALA A | 24 | -16.772 | 62.334 | 2.176  | 1.00 | 52.15 |
| ATOM | 152 | O   | ALA A | 24 | -15.617 | 61.905 | 2.114  | 1.00 | 55.14 |
| ATOM | 153 | N   | LYS A | 25 | -17.097 | 63.443 | 2.835  | 1.00 | 46.23 |
| ATOM | 154 | CA  | LYS A | 25 | -16.087 | 64.230 | 3.516  | 1.00 | 42.19 |
| ATOM | 155 | CB  | LYS A | 25 | -16.690 | 65.505 | 4.112  | 1.00 | 38.59 |
| ATOM | 156 | CG  | LYS A | 25 | -16.655 | 66.663 | 3.149  | 1.00 | 33.56 |
| ATOM | 157 | CD  | LYS A | 25 | -17.022 | 67.980 | 3.806  | 1.00 | 35.11 |
| ATOM | 158 | CE  | LYS A | 25 | -18.525 | 68.172 | 3.890  | 1.00 | 37.82 |
| ATOM | 159 | NZ  | LYS A | 25 | -18.878 | 69.562 | 4.275  | 1.00 | 39.00 |
| ATOM | 160 | C   | LYS A | 25 | -15.406 | 63.406 | 4.593  | 1.00 | 43.50 |
| ATOM | 161 | O   | LYS A | 25 | -14.186 | 63.378 | 4.688  | 1.00 | 45.05 |
| ATOM | 162 | N   | MET A | 26 | -16.189 | 62.680 | 5.368  | 1.00 | 46.05 |
| ATOM | 163 | CA  | MET A | 26 | -15.599 | 61.872 | 6.424  | 1.00 | 51.52 |
| ATOM | 164 | CB  | MET A | 26 | -16.674 | 61.263 | 7.306  | 1.00 | 58.77 |
| ATOM | 165 | CG  | MET A | 26 | -17.065 | 62.138 | 8.503  | 1.00 | 68.62 |
| ATOM | 166 | SD  | MET A | 26 | -15.776 | 62.302 | 9.788  | 1.00 | 75.98 |
| ATOM | 167 | CE  | MET A | 26 | -15.385 | 60.571 | 10.146 | 1.00 | 72.86 |
| ATOM | 168 | C   | MET A | 26 | -14.740 | 60.785 | 5.816  | 1.00 | 49.91 |
| ATOM | 169 | O   | MET A | 26 | -13.709 | 60.391 | 6.395  | 1.00 | 49.46 |
| ATOM | 170 | N   | ARG A | 27 | -15.148 | 60.307 | 4.645  | 1.00 | 50.27 |
| ATOM | 171 | CA  | ARG A | 27 | -14.407 | 59.273 | 3.942  | 1.00 | 51.72 |
| ATOM | 172 | CB  | ARG A | 27 | -15.141 | 58.858 | 2.662  | 1.00 | 59.72 |
| ATOM | 173 | CG  | ARG A | 27 | -15.819 | 57.511 | 2.736  | 1.00 | 70.60 |
| ATOM | 174 | CD  | ARG A | 27 | -16.315 | 57.084 | 1.365  | 1.00 | 80.78 |
| ATOM | 175 | NE  | ARG A | 27 | -17.703 | 57.450 | 1.123  | 1.00 | 88.62 |
| ATOM | 176 | CZ  | ARG A | 27 | -18.115 | 58.133 | 0.056  | 1.00 | 93.71 |
| ATOM | 177 | NH1 | ARG A | 27 | -17.243 | 58.547 | -0.867 | 1.00 | 96.83 |
| ATOM | 178 | NH2 | ARG A | 27 | -19.414 | 58.338 | -0.135 | 1.00 | 97.09 |
| ATOM | 179 | C   | ARG A | 27 | -13.026 | 59.802 | 3.585  | 1.00 | 48.21 |
| ATOM | 180 | O   | ARG A | 27 | -12.030 | 59.115 | 3.794  | 1.00 | 49.76 |
| ATOM | 181 | N   | VAL A | 28 | -12.977 | 61.018 | 3.040  | 1.00 | 44.43 |
| ATOM | 182 | CA  | VAL A | 28 | -11.705 | 61.637 | 2.669  | 1.00 | 40.68 |
| ATOM | 183 | CB  | VAL A | 28 | -11.896 | 63.013 | 1.989  | 1.00 | 40.13 |
| ATOM | 184 | CG1 | VAL A | 28 | -10.540 | 63.639 | 1.672  | 1.00 | 40.08 |
| ATOM | 185 | CG2 | VAL A | 28 | -12.684 | 62.844 | 0.709  | 1.00 | 39.09 |
| ATOM | 186 | C   | VAL A | 28 | -10.868 | 61.798 | 3.922  | 1.00 | 41.23 |
| ATOM | 187 | O   | VAL A | 28 | -9.706  | 61.381 | 3.963  | 1.00 | 41.90 |
| ATOM | 188 | N   | ALA A | 29 | -11.510 | 62.271 | 4.981  | 1.00 | 40.14 |
| ATOM | 189 | CA  | ALA A | 29 | -10.854 | 62.492 | 6.255  | 1.00 | 39.42 |
| ATOM | 190 | CB  | ALA A | 29 | -11.873 | 62.936 | 7.274  | 1.00 | 40.42 |
| ATOM | 191 | C   | ALA A | 29 | -10.131 | 61.242 | 6.731  | 1.00 | 41.63 |
| ATOM | 192 | O   | ALA A | 29 | -8.963  | 61.307 | 7.119  | 1.00 | 42.66 |
| ATOM | 193 | N   | GLN A | 30 | -10.803 | 60.099 | 6.666  | 1.00 | 44.91 |
| ATOM | 194 | CA  | GLN A | 30 | -10.201 | 58.848 | 7.106  | 1.00 | 48.27 |
| ATOM | 195 | CB  | GLN A | 30 | -11.203 | 57.702 | 6.971  | 1.00 | 54.77 |
| ATOM | 196 | CG  | GLN A | 30 | -12.400 | 57.837 | 7.901  | 1.00 | 67.39 |
| ATOM | 197 | CD  | GLN A | 30 | -13.579 | 56.964 | 7.495  | 1.00 | 75.12 |
| ATOM | 198 | OE1 | GLN A | 30 | -13.471 | 56.115 | 6.605  | 1.00 | 77.42 |
| ATOM | 199 | NE2 | GLN A | 30 | -14.724 | 57.189 | 8.136  | 1.00 | 79.26 |
| ATOM | 200 | C   | GLN A | 30 | -8.930  | 58.544 | 6.328  | 1.00 | 47.85 |
| ATOM | 201 | O   | GLN A | 30 | -7.933  | 58.099 | 6.898  | 1.00 | 49.06 |
| ATOM | 202 | N   | GLN A | 31 | -8.972  | 58.807 | 5.025  | 1.00 | 45.74 |
| ATOM | 203 | CA  | GLN A | 31 | -7.820  | 58.573 | 4.164  | 1.00 | 42.76 |
| ATOM | 204 | CB  | GLN A | 31 | -8.188  | 58.781 | 2.701  | 1.00 | 40.15 |
| ATOM | 205 | CG  | GLN A | 31 | -9.129  | 57.723 | 2.175  | 1.00 | 43.01 |
| ATOM | 206 | CD  | GLN A | 31 | -9.468  | 57.922 | 0.715  | 1.00 | 48.15 |
| ATOM | 207 | OE1 | GLN A | 31 | -8.717  | 57.518 | -0.166 | 1.00 | 52.25 |
| ATOM | 208 | NE2 | GLN A | 31 | -10.609 | 58.541 | 0.449  | 1.00 | 55.93 |
| ATOM | 209 | C   | GLN A | 31 | -6.675  | 59.494 | 4.568  | 1.00 | 41.22 |
| ATOM | 210 | O   | GLN A | 31 | -5.547  | 59.042 | 4.765  | 1.00 | 43.52 |
| ATOM | 211 | N   | ILE A | 32 | -6.977  | 60.778 | 4.732  | 1.00 | 37.48 |
| ATOM | 212 | CA  | ILE A | 32 | -5.972  | 61.746 | 5.138  | 1.00 | 31.13 |
| ATOM | 213 | CB  | ILE A | 32 | -6.581  | 63.140 | 5.280  | 1.00 | 26.04 |
| ATOM | 214 | CG2 | ILE A | 32 | -5.615  | 64.067 | 5.954  | 1.00 | 22.19 |
| ATOM | 215 | CG1 | ILE A | 32 | -6.987  | 63.663 | 3.904  | 1.00 | 25.80 |

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|      |     |     |       |    |        |        |        |      |       |
|------|-----|-----|-------|----|--------|--------|--------|------|-------|
| ATOM | 216 | CD1 | ILE A | 32 | -7.608 | 65.039 | 3.924  | 1.00 | 27.42 |
| ATOM | 217 | C   | ILE A | 32 | -5.343 | 61.308 | 6.458  | 1.00 | 34.56 |
| ATOM | 218 | O   | ILE A | 32 | -4.123 | 61.345 | 6.606  | 1.00 | 38.92 |
| ATOM | 219 | N   | ASP A | 33 | -6.169 | 60.833 | 7.387  | 1.00 | 36.94 |
| ATOM | 220 | CA  | ASP A | 33 | -5.684 | 60.375 | 8.689  | 1.00 | 38.24 |
| ATOM | 221 | CB  | ASP A | 33 | -6.850 | 59.928 | 9.588  | 1.00 | 44.05 |
| ATOM | 222 | CG  | ASP A | 33 | -6.380 | 59.328 | 10.930 | 1.00 | 47.52 |
| ATOM | 223 | OD1 | ASP A | 33 | -5.824 | 60.066 | 11.773 | 1.00 | 44.85 |
| ATOM | 224 | OD2 | ASP A | 33 | -6.583 | 58.111 | 11.149 | 1.00 | 46.89 |
| ATOM | 225 | C   | ASP A | 33 | -4.695 | 59.233 | 8.529  | 1.00 | 36.71 |
| ATOM | 226 | O   | ASP A | 33 | -3.654 | 59.209 | 9.182  | 1.00 | 39.40 |
| ATOM | 227 | N   | ALA A | 34 | -5.012 | 58.285 | 7.658  | 1.00 | 33.88 |
| ATOM | 228 | CA  | ALA A | 34 | -4.129 | 57.148 | 7.445  | 1.00 | 34.39 |
| ATOM | 229 | CB  | ALA A | 34 | -4.808 | 56.126 | 6.579  | 1.00 | 35.43 |
| ATOM | 230 | C   | ALA A | 34 | -2.783 | 57.560 | 6.841  | 1.00 | 38.07 |
| ATOM | 231 | O   | ALA A | 34 | -1.728 | 57.088 | 7.280  | 1.00 | 42.04 |
| ATOM | 232 | N   | ALA A | 35 | -2.817 | 58.454 | 5.851  | 1.00 | 37.24 |
| ATOM | 233 | CA  | ALA A | 35 | -1.596 | 58.933 | 5.197  | 1.00 | 34.56 |
| ATOM | 234 | CB  | ALA A | 35 | -1.941 | 59.864 | 4.054  | 1.00 | 31.14 |
| ATOM | 235 | C   | ALA A | 35 | -0.697 | 59.648 | 6.189  | 1.00 | 33.05 |
| ATOM | 236 | O   | ALA A | 35 | 0.485  | 59.347 | 6.295  | 1.00 | 36.62 |
| ATOM | 237 | N   | SER A | 36 | -1.276 | 60.589 | 6.923  | 1.00 | 32.76 |
| ATOM | 238 | CA  | SER A | 36 | -0.556 | 61.369 | 7.919  | 1.00 | 35.08 |
| ATOM | 239 | CB  | SER A | 36 | -1.503 | 62.396 | 8.544  | 1.00 | 30.17 |
| ATOM | 240 | OG  | SER A | 36 | -2.181 | 63.133 | 7.539  | 1.00 | 33.36 |
| ATOM | 241 | C   | SER A | 36 | 0.054  | 60.506 | 9.021  | 1.00 | 39.08 |
| ATOM | 242 | O   | SER A | 36 | 0.950  | 60.955 | 9.750  | 1.00 | 41.57 |
| ATOM | 243 | N   | ARG A | 37 | -0.456 | 59.288 | 9.172  | 1.00 | 38.47 |
| ATOM | 244 | CA  | ARG A | 37 | 0.053  | 58.394 | 10.191 | 1.00 | 38.11 |
| ATOM | 245 | CB  | ARG A | 37 | -1.095 | 57.702 | 10.908 | 1.00 | 40.18 |
| ATOM | 246 | CG  | ARG A | 37 | -1.866 | 58.642 | 11.805 | 1.00 | 47.64 |
| ATOM | 247 | CD  | ARG A | 37 | -3.157 | 58.021 | 12.262 | 1.00 | 55.80 |
| ATOM | 248 | NE  | ARG A | 37 | -2.923 | 56.776 | 12.976 | 1.00 | 66.31 |
| ATOM | 249 | C2  | ARG A | 37 | -3.859 | 55.865 | 13.219 | 1.00 | 72.83 |
| ATOM | 250 | NH1 | ARG A | 37 | -5.109 | 56.056 | 12.805 | 1.00 | 73.10 |
| ATOM | 251 | NH2 | ARG A | 37 | -3.538 | 54.753 | 13.872 | 1.00 | 79.16 |
| ATOM | 252 | C   | ARG A | 37 | 1.035  | 57.393 | 9.627  | 1.00 | 38.74 |
| ATOM | 253 | O   | ARG A | 37 | 1.677  | 56.672 | 10.380 | 1.00 | 40.61 |
| ATOM | 254 | N   | ASP A | 38 | 1.151  | 57.349 | 8.305  | 1.00 | 40.43 |
| ATOM | 255 | CA  | ASP A | 38 | 2.086  | 56.440 | 7.658  | 1.00 | 41.47 |
| ATOM | 256 | CB  | ASP A | 38 | 1.435  | 55.783 | 6.437  | 1.00 | 49.45 |
| ATOM | 257 | CG  | ASP A | 38 | 2.199  | 54.556 | 5.951  | 1.00 | 58.59 |
| ATOM | 258 | OD1 | ASP A | 38 | 2.821  | 53.855 | 6.784  | 1.00 | 62.36 |
| ATOM | 259 | OD2 | ASP A | 38 | 2.162  | 54.281 | 4.732  | 1.00 | 62.50 |
| ATOM | 260 | C   | ASP A | 38 | 3.351  | 57.218 | 7.262  | 1.00 | 40.48 |
| ATOM | 261 | O   | ASP A | 38 | 4.213  | 57.461 | 8.105  | 1.00 | 36.69 |
| ATOM | 262 | N   | THR A | 39 | 3.449  | 57.618 | 5.991  | 1.00 | 41.01 |
| ATOM | 263 | CA  | THR A | 39 | 4.597  | 58.376 | 5.480  | 1.00 | 39.22 |
| ATOM | 264 | CB  | THR A | 39 | 4.675  | 58.298 | 3.948  | 1.00 | 39.18 |
| ATOM | 265 | OG1 | THR A | 39 | 3.363  | 58.473 | 3.393  | 1.00 | 44.29 |
| ATOM | 266 | CG2 | THR A | 39 | 5.221  | 56.968 | 3.519  | 1.00 | 43.28 |
| ATOM | 267 | C   | THR A | 39 | 4.497  | 59.847 | 5.850  | 1.00 | 37.79 |
| ATOM | 268 | O   | THR A | 39 | 5.505  | 60.538 | 5.973  | 1.00 | 41.79 |
| ATOM | 269 | N   | GLY A | 40 | 3.268  | 60.323 | 5.993  | 1.00 | 35.69 |
| ATOM | 270 | CA  | GLY A | 40 | 3.038  | 61.711 | 6.336  | 1.00 | 34.49 |
| ATOM | 271 | C   | GLY A | 40 | 2.842  | 62.524 | 5.078  | 1.00 | 32.99 |
| ATOM | 272 | O   | GLY A | 40 | 2.649  | 63.735 | 5.153  | 1.00 | 35.66 |
| ATOM | 273 | N   | PHE A | 41 | 2.867  | 61.842 | 3.932  | 1.00 | 30.35 |
| ATOM | 274 | CA  | PHE A | 41 | 2.713  | 62.465 | 2.617  | 1.00 | 23.42 |
| ATOM | 275 | CB  | PHE A | 41 | 3.986  | 62.260 | 1.780  | 1.00 | 19.36 |
| ATOM | 276 | CG  | PHE A | 41 | 5.094  | 63.225 | 2.094  | 1.00 | 19.44 |
| ATOM | 277 | CD1 | PHE A | 41 | 6.079  | 62.899 | 3.013  | 1.00 | 20.61 |
| ATOM | 278 | CD2 | PHE A | 41 | 5.161  | 64.455 | 1.454  | 1.00 | 21.76 |
| ATOM | 279 | CE1 | PHE A | 41 | 7.120  | 63.790 | 3.292  | 1.00 | 19.48 |
| ATOM | 280 | CE2 | PHE A | 41 | 6.192  | 65.350 | 1.723  | 1.00 | 20.92 |
| ATOM | 281 | CZ  | PHE A | 41 | 7.173  | 65.018 | 2.642  | 1.00 | 26.83 |
| ATOM | 282 | C   | PHE A | 41 | 1.558  | 61.855 | 1.840  | 1.00 | 33.65 |
| ATOM | 283 | O   | PHE A | 41 | 1.269  | 60.671 | 1.988  | 1.00 | 29.43 |
| ATOM | 284 | N   | PHE A | 42 | 0.900  | 62.662 | 1.016  | 1.00 | 28.45 |
| ATOM | 285 | CA  | PHE A | 42 | -0.179 | 62.172 | 0.171  | 1.00 | 28.60 |
| ATOM | 286 | CB  | PHE A | 42 | -1.473 | 61.872 | 0.953  | 1.00 | 26.89 |
| ATOM | 287 | CG  | PHE A | 42 | -2.292 | 63.083 | 1.332  | 1.00 | 26.83 |
| ATOM | 288 | CD1 | PHE A | 42 | -3.186 | 63.655 | 0.431  | 1.00 | 26.89 |

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|      |     |     |       |    |         |        |         |      |       |
|------|-----|-----|-------|----|---------|--------|---------|------|-------|
| ATOM | 289 | CD2 | PHE A | 42 | -2.218  | 63.612 | 2.613   | 1.00 | 28.60 |
| ATOM | 290 | CE1 | PHE A | 42 | -3.998  | 64.734 | 0.803   | 1.00 | 22.24 |
| ATOM | 291 | CE2 | PHE A | 42 | -3.030  | 64.692 | 2.993   | 1.00 | 28.04 |
| ATOM | 292 | CZ  | PHE A | 42 | -3.919  | 65.249 | 2.081   | 1.00 | 22.14 |
| ATOM | 293 | C   | PHE A | 42 | -0.416  | 63.122 | -0.979  | 1.00 | 30.71 |
| ATOM | 294 | O   | PHE A | 42 | -0.046  | 64.297 | -0.908  | 1.00 | 32.62 |
| ATOM | 295 | N   | TYR A | 43 | -0.911  | 62.580 | -2.084  | 1.00 | 31.35 |
| ATOM | 296 | CA  | TYR A | 43 | -1.200  | 63.386 | -3.257  | 1.00 | 27.25 |
| ATOM | 297 | CB  | TYR A | 43 | -0.851  | 62.641 | -4.556  | 1.00 | 25.54 |
| ATOM | 298 | CG  | TYR A | 43 | 0.573   | 62.844 | -5.054  | 1.00 | 21.56 |
| ATOM | 299 | CD1 | TYR A | 43 | 1.524   | 61.841 | -4.942  | 1.00 | 19.07 |
| ATOM | 300 | CE1 | TYR A | 43 | 2.835   | 62.034 | -5.386  | 1.00 | 17.94 |
| ATOM | 301 | CD2 | TYR A | 43 | 0.966   | 64.047 | -5.628  | 1.00 | 23.58 |
| ATOM | 302 | CE2 | TYR A | 43 | 2.272   | 64.246 | -6.068  | 1.00 | 15.91 |
| ATOM | 303 | CZ  | TYR A | 43 | 3.198   | 63.241 | -5.946  | 1.00 | 16.09 |
| ATOM | 304 | OH  | TYR A | 43 | -2.673  | 63.735 | -6.375  | 1.00 | 15.37 |
| ATOM | 305 | C   | TYR A | 43 | -3.528  | 62.861 | -3.249  | 1.00 | 29.51 |
| ATOM | 306 | O   | TYR A | 43 | -2.960  | 65.026 | -3.163  | 1.00 | 26.39 |
| ATOM | 307 | N   | ALA A | 44 | -4.327  | 65.497 | -3.252  | 1.00 | 32.50 |
| ATOM | 308 | CA  | ALA A | 44 | -4.448  | 66.834 | -3.290  | 1.00 | 32.14 |
| ATOM | 309 | CB  | ALA A | 44 | -4.580  | 65.658 | -2.586  | 1.00 | 31.97 |
| ATOM | 310 | C   | ALA A | 44 | -3.968  | 66.506 | -4.769  | 1.00 | 33.03 |
| ATOM | 311 | O   | ALA A | 44 | -5.416  | 64.790 | -5.414  | 1.00 | 33.76 |
| ATOM | 312 | N   | VAL A | 45 | -5.741  | 64.824 | -5.317  | 1.00 | 35.03 |
| ATOM | 313 | CA  | VAL A | 45 | -5.548  | 63.440 | -6.729  | 1.00 | 36.59 |
| ATOM | 314 | CB  | VAL A | 45 | -6.543  | 62.454 | -7.353  | 1.00 | 40.19 |
| ATOM | 315 | CG1 | VAL A | 45 | -6.656  | 63.525 | -6.770  | 1.00 | 47.08 |
| ATOM | 316 | CG2 | VAL A | 45 | -7.184  | 65.291 | -8.861  | 1.00 | 36.63 |
| ATOM | 317 | C   | VAL A | 45 | -7.960  | 65.177 | -9.144  | 1.00 | 42.25 |
| ATOM | 318 | O   | VAL A | 45 | -7.538  | 65.823 | -9.517  | 1.00 | 36.71 |
| ATOM | 319 | N   | ASN A | 46 | -8.883  | 66.349 | -8.034  | 1.00 | 35.51 |
| ATOM | 320 | CA  | ASN A | 46 | -9.956  | 65.320 | -8.294  | 1.00 | 42.00 |
| ATOM | 321 | CB  | ASN A | 46 | -10.436 | 64.547 | -7.942  | 1.00 | 51.81 |
| ATOM | 322 | CG  | ASN A | 46 | -11.513 | 64.813 | -9.671  | 1.00 | 58.83 |
| ATOM | 323 | OD1 | ASN A | 46 | -9.641  | 63.582 | -9.588  | 1.00 | 54.06 |
| ATOM | 324 | ND2 | ASN A | 46 | -9.121  | 67.618 | -7.494  | 1.00 | 32.25 |
| ATOM | 325 | C   | ASN A | 46 | -10.206 | 67.848 | -6.996  | 1.00 | 35.38 |
| ATOM | 326 | O   | ASN A | 46 | -8.093  | 68.452 | -7.409  | 1.00 | 34.05 |
| ATOM | 327 | N   | HIS A | 47 | -8.106  | 69.718 | -6.659  | 1.00 | 34.39 |
| ATOM | 328 | CA  | HIS A | 47 | -6.674  | 70.088 | -6.306  | 1.00 | 29.40 |
| ATOM | 329 | CB  | HIS A | 47 | -5.716  | 69.842 | -7.425  | 1.00 | 26.18 |
| ATOM | 330 | CG  | HIS A | 47 | -4.906  | 68.789 | -7.686  | 1.00 | 27.13 |
| ATOM | 331 | CD2 | HIS A | 47 | -5.573  | 70.709 | -8.486  | 1.00 | 29.56 |
| ATOM | 332 | ND1 | HIS A | 47 | -4.717  | 70.199 | -9.355  | 1.00 | 29.92 |
| ATOM | 333 | CE1 | HIS A | 47 | -4.299  | 69.034 | -8.894  | 1.00 | 29.91 |
| ATOM | 334 | NE2 | HIS A | 47 | -8.740  | 70.890 | -7.397  | 1.00 | 35.30 |
| ATOM | 335 | C   | HIS A | 47 | -8.889  | 71.972 | -6.825  | 1.00 | 36.82 |
| ATOM | 336 | O   | HIS A | 47 | -8.955  | 70.710 | -8.700  | 1.00 | 36.56 |
| ATOM | 337 | N   | GLY A | 48 | -9.578  | 71.732 | -9.528  | 1.00 | 37.05 |
| ATOM | 338 | CA  | GLY A | 48 | -8.759  | 72.959 | -9.879  | 1.00 | 40.00 |
| ATOM | 339 | C   | GLY A | 48 | -9.321  | 74.004 | -10.196 | 1.00 | 46.68 |
| ATOM | 340 | O   | GLY A | 48 | -7.440  | 72.819 | -9.913  | 1.00 | 37.89 |
| ATOM | 341 | N   | ILE A | 49 | -6.568  | 73.948 | -10.220 | 1.00 | 36.05 |
| ATOM | 342 | CA  | ILE A | 49 | -5.546  | 74.191 | -9.082  | 1.00 | 31.81 |
| ATOM | 343 | CB  | ILE A | 49 | -4.522  | 75.255 | -9.488  | 1.00 | 28.58 |
| ATOM | 344 | CG2 | ILE A | 49 | -6.287  | 74.596 | -7.807  | 1.00 | 29.79 |
| ATOM | 345 | CG1 | ILE A | 49 | -5.425  | 74.629 | -6.574  | 1.00 | 32.52 |
| ATOM | 346 | CD1 | ILE A | 49 | -5.815  | 73.686 | -11.514 | 1.00 | 38.13 |
| ATOM | 347 | C   | ILE A | 49 | -5.297  | 72.581 | -11.707 | 1.00 | 38.18 |
| ATOM | 348 | O   | ILE A | 49 | -5.749  | 74.701 | -12.383 | 1.00 | 38.60 |
| ATOM | 349 | N   | ASN A | 50 | -5.050  | 74.603 | -13.663 | 1.00 | 38.30 |
| ATOM | 350 | CA  | ASN A | 50 | -5.453  | 75.726 | -14.619 | 1.00 | 42.37 |
| ATOM | 351 | CB  | ASN A | 50 | -4.920  | 75.502 | -16.033 | 1.00 | 46.03 |
| ATOM | 352 | CG  | ASN A | 50 | -4.258  | 74.496 | -16.314 | 1.00 | 46.67 |
| ATOM | 353 | OD1 | ASN A | 50 | -5.195  | 76.445 | -16.922 | 1.00 | 49.68 |
| ATOM | 354 | ND2 | ASN A | 50 | -3.544  | 74.614 | -13.439 | 1.00 | 38.19 |
| ATOM | 355 | C   | ASN A | 50 | -2.853  | 75.631 | -13.581 | 1.00 | 36.43 |
| ATOM | 356 | O   | ASN A | 50 | -3.064  | 73.436 | -13.086 | 1.00 | 39.42 |
| ATOM | 357 | N   | VAL A | 51 | -1.676  | 73.165 | -12.786 | 1.00 | 38.94 |
| ATOM | 358 | CA  | VAL A | 51 | -1.582  | 71.734 | -12.182 | 1.00 | 36.89 |
| ATOM | 359 | CB  | VAL A | 51 | -0.757  | 70.802 | -13.040 | 1.00 | 39.25 |
| ATOM | 360 | CG1 | VAL A | 51 | -1.103  | 71.797 | -10.756 | 1.00 | 37.13 |
| ATOM | 361 | CG2 | VAL A | 51 | -1.103  |        |         |      |       |

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|      |     |     |       |    |        |        |         |      |       |
|------|-----|-----|-------|----|--------|--------|---------|------|-------|
| ATOM | 362 | C   | VAL A | 51 | -0.804 | 73.346 | -14.025 | 1.00 | 40.42 |
| ATOM | 363 | O   | VAL A | 51 | 0.370  | 73.688 | -13.923 | 1.00 | 40.47 |
| ATOM | 364 | N   | GLN A | 52 | -1.404 | 73.193 | -15.198 | 1.00 | 43.48 |
| ATOM | 365 | CA  | GLN A | 52 | -0.658 | 73.335 | -16.439 | 1.00 | 46.46 |
| ATOM | 366 | CB  | GLN A | 52 | -1.461 | 72.753 | -17.607 | 1.00 | 54.80 |
| ATOM | 367 | CG  | GLN A | 52 | -1.828 | 71.265 | -17.427 | 1.00 | 64.12 |
| ATOM | 368 | CD  | GLN A | 52 | -0.603 | 70.340 | -17.338 | 1.00 | 70.98 |
| ATOM | 369 | OE1 | GLN A | 52 | 0.494  | 70.696 | -17.774 | 1.00 | 73.27 |
| ATOM | 370 | NE2 | GLN A | 52 | -0.799 | 69.140 | -16.788 | 1.00 | 71.68 |
| ATOM | 371 | C   | GLN A | 52 | -0.250 | 74.787 | -16.694 | 1.00 | 42.90 |
| ATOM | 372 | O   | GLN A | 52 | 0.932  | 75.081 | -16.876 | 1.00 | 42.08 |
| ATOM | 373 | N   | ARG A | 53 | -1.212 | 75.704 | -16.649 | 1.00 | 40.10 |
| ATOM | 374 | CA  | ARG A | 53 | -0.902 | 77.119 | -16.860 | 1.00 | 40.21 |
| ATOM | 375 | CB  | ARG A | 53 | -2.161 | 77.981 | -16.766 | 1.00 | 39.62 |
| ATOM | 376 | CG  | ARG A | 53 | -1.896 | 79.468 | -16.979 | 1.00 | 46.56 |
| ATOM | 377 | CD  | ARG A | 53 | -3.084 | 80.302 | -16.558 | 1.00 | 55.52 |
| ATOM | 378 | NE  | ARG A | 53 | -3.456 | 80.002 | -15.180 | 1.00 | 69.72 |
| ATOM | 379 | CZ  | ARG A | 53 | -4.707 | 79.854 | -14.750 | 1.00 | 75.43 |
| ATOM | 380 | NH1 | ARG A | 53 | -5.728 | 79.988 | -15.589 | 1.00 | 79.20 |
| ATOM | 381 | NH2 | ARG A | 53 | -4.936 | 79.529 | -13.485 | 1.00 | 80.30 |
| ATOM | 382 | C   | ARG A | 53 | 0.112  | 77.592 | -15.818 | 1.00 | 40.89 |
| ATOM | 383 | O   | ARG A | 53 | 0.967  | 78.436 | -16.103 | 1.00 | 42.68 |
| ATOM | 384 | N   | LEU A | 54 | 0.015  | 77.025 | -14.617 | 1.00 | 40.83 |
| ATOM | 385 | CA  | LEU A | 54 | 0.906  | 77.354 | -13.513 | 1.00 | 36.14 |
| ATOM | 386 | CB  | LEU A | 54 | 0.481  | 76.583 | -12.263 | 1.00 | 36.52 |
| ATOM | 387 | CG  | LEU A | 54 | 1.431  | 76.620 | -11.068 | 1.00 | 35.31 |
| ATOM | 388 | CD1 | LEU A | 54 | 1.581  | 78.057 | -10.586 | 1.00 | 33.45 |
| ATOM | 389 | CD2 | LEU A | 54 | 0.904  | 75.710 | -9.969  | 1.00 | 36.19 |
| ATOM | 390 | C   | LEU A | 54 | 2.380  | 77.073 | -13.829 | 1.00 | 36.31 |
| ATOM | 391 | O   | LEU A | 54 | 3.231  | 77.935 | -13.618 | 1.00 | 37.16 |
| ATOM | 392 | N   | SER A | 55 | 2.695  | 75.883 | -14.335 | 1.00 | 34.98 |
| ATOM | 393 | CA  | SER A | 55 | 4.090  | 75.558 | -14.645 | 1.00 | 36.10 |
| ATOM | 394 | CB  | SER A | 55 | 4.261  | 74.066 | -14.929 | 1.00 | 32.09 |
| ATOM | 395 | OG  | SER A | 55 | 3.071  | 73.521 | -15.455 | 1.00 | 41.05 |
| ATOM | 396 | C   | SER A | 55 | 4.618  | 76.377 | -15.804 | 1.00 | 37.67 |
| ATOM | 397 | O   | SER A | 55 | 5.789  | 76.752 | -15.825 | 1.00 | 41.07 |
| ATOM | 398 | N   | GLN A | 56 | 3.740  | 76.688 | -16.744 | 1.00 | 37.35 |
| ATOM | 399 | CA  | GLN A | 56 | 4.105  | 77.460 | -17.919 | 1.00 | 38.51 |
| ATOM | 400 | CB  | GLN A | 56 | 2.940  | 77.439 | -18.902 | 1.00 | 46.09 |
| ATOM | 401 | CG  | GLN A | 56 | 3.138  | 78.188 | -20.191 | 1.00 | 58.62 |
| ATOM | 402 | CD  | GLN A | 56 | 1.811  | 78.422 | -20.902 | 1.00 | 71.60 |
| ATOM | 403 | OE1 | GLN A | 56 | 1.007  | 77.494 | -21.071 | 1.00 | 75.28 |
| ATOM | 404 | NE2 | GLN A | 56 | 1.560  | 79.672 | -21.296 | 1.00 | 74.89 |
| ATOM | 405 | C   | GLN A | 56 | 4.496  | 78.893 | -17.560 | 1.00 | 36.41 |
| ATOM | 406 | O   | GLN A | 56 | 5.611  | 79.312 | -17.848 | 1.00 | 35.97 |
| ATOM | 407 | N   | LYS A | 57 | 3.599  | 79.629 | -16.905 | 1.00 | 35.19 |
| ATOM | 408 | CA  | LYS A | 57 | 3.869  | 81.015 | -16.514 | 1.00 | 34.22 |
| ATOM | 409 | CB  | LYS A | 57 | 2.710  | 81.567 | -15.693 | 1.00 | 35.10 |
| ATOM | 410 | CG  | LYS A | 57 | 1.443  | 81.768 | -16.469 | 1.00 | 41.47 |
| ATOM | 411 | CD  | LYS A | 57 | 1.644  | 82.849 | -17.492 | 1.00 | 49.86 |
| ATOM | 412 | CE  | LYS A | 57 | 0.507  | 82.868 | -18.477 | 1.00 | 58.96 |
| ATOM | 413 | NZ  | LYS A | 57 | 0.740  | 83.914 | -19.507 | 1.00 | 67.82 |
| ATOM | 414 | C   | LYS A | 57 | 5.147  | 81.106 | -15.691 | 1.00 | 36.94 |
| ATOM | 415 | O   | LYS A | 57 | 5.963  | 82.014 | -15.875 | 1.00 | 38.60 |
| ATOM | 416 | N   | THR A | 58 | 5.277  | 80.172 | -14.753 | 1.00 | 37.65 |
| ATOM | 417 | CA  | THR A | 58 | 6.426  | 80.066 | -13.865 | 1.00 | 35.48 |
| ATOM | 418 | CB  | THR A | 58 | 6.215  | 78.911 | -12.846 | 1.00 | 36.09 |
| ATOM | 419 | OG1 | THR A | 58 | 5.257  | 79.317 | -11.862 | 1.00 | 30.91 |
| ATOM | 420 | CG2 | THR A | 58 | 7.503  | 78.549 | -12.142 | 1.00 | 43.44 |
| ATOM | 421 | C   | THR A | 58 | 7.696  | 79.833 | -14.665 | 1.00 | 35.79 |
| ATOM | 422 | O   | THR A | 58 | 8.686  | 80.531 | -14.463 | 1.00 | 37.07 |
| ATOM | 423 | N   | LYS A | 59 | 7.667  | 78.865 | -15.577 | 1.00 | 38.20 |
| ATOM | 424 | CA  | LYS A | 59 | 8.832  | 78.573 | -16.397 | 1.00 | 40.23 |
| ATOM | 425 | CB  | LYS A | 59 | 8.540  | 77.444 | -17.391 | 1.00 | 46.70 |
| ATOM | 426 | CG  | LYS A | 59 | 9.744  | 77.071 | -18.254 | 1.00 | 58.45 |
| ATOM | 427 | CD  | LYS A | 59 | 9.534  | 75.783 | -19.053 | 1.00 | 69.21 |
| ATOM | 428 | CE  | LYS A | 59 | 10.831 | 75.350 | -19.769 | 1.00 | 76.48 |
| ATOM | 429 | NZ  | LYS A | 59 | 10.728 | 74.041 | -20.510 | 1.00 | 75.66 |
| ATOM | 430 | C   | LYS A | 59 | 9.199  | 79.846 | -17.134 | 1.00 | 40.20 |
| ATOM | 431 | O   | LYS A | 59 | 10.364 | 80.239 | -17.167 | 1.00 | 41.89 |
| ATOM | 432 | N   | GLU A | 60 | 8.186  | 80.531 | -17.653 | 1.00 | 41.30 |
| ATOM | 433 | CA  | GLU A | 60 | 8.395  | 81.777 | -18.379 | 1.00 | 42.90 |
| ATOM | 434 | CB  | GLU A | 60 | 7.059  | 82.362 | -18.851 | 1.00 | 50.15 |

|      |     |     |       |    |        |        |         |      |       |
|------|-----|-----|-------|----|--------|--------|---------|------|-------|
| ATOM | 435 | CG  | GLU A | 60 | 6.405  | 81.626 | -20.026 | 1.00 | 57.31 |
| ATOM | 436 | CD  | GLU A | 60 | 5.215  | 82.383 | -20.605 | 1.00 | 63.82 |
| ATOM | 437 | OE1 | GLU A | 60 | 4.233  | 81.733 | -21.027 | 1.00 | 68.21 |
| ATOM | 438 | OE2 | GLU A | 60 | 5.259  | 83.633 | -20.644 | 1.00 | 67.21 |
| ATOM | 439 | C   | GLU A | 60 | 9.115  | 82.773 | -17.484 | 1.00 | 39.96 |
| ATOM | 440 | O   | GLU A | 60 | 10.147 | 83.324 | -17.859 | 1.00 | 42.99 |
| ATOM | 441 | N   | PHE A | 61 | 8.604  | 82.949 | -16.274 | 1.00 | 35.82 |
| ATOM | 442 | CA  | PHE A | 61 | 9.208  | 83.874 | -15.325 | 1.00 | 34.12 |
| ATOM | 443 | CB  | PHE A | 61 | 8.466  | 83.810 | -13.978 | 1.00 | 30.54 |
| ATOM | 444 | CG  | PHE A | 61 | 9.039  | 84.718 | -12.918 | 1.00 | 25.45 |
| ATOM | 445 | CD1 | PHE A | 61 | 8.905  | 86.093 | -13.013 | 1.00 | 20.40 |
| ATOM | 446 | CD2 | PHE A | 61 | 9.730  | 84.193 | -11.835 | 1.00 | 23.25 |
| ATOM | 447 | CE1 | PHE A | 61 | 9.449  | 86.928 | -12.053 | 1.00 | 19.57 |
| ATOM | 448 | CE2 | PHE A | 61 | 10.277 | 85.026 | -10.875 | 1.00 | 22.69 |
| ATOM | 449 | CZ  | PHE A | 61 | 10.133 | 86.399 | -10.989 | 1.00 | 17.25 |
| ATOM | 450 | C   | PHE A | 61 | 10.710 | 83.620 | -15.115 | 1.00 | 32.38 |
| ATOM | 451 | O   | PHE A | 61 | 11.536 | 84.499 | -15.353 | 1.00 | 30.20 |
| ATOM | 452 | N   | HIS A | 62 | 11.064 | 82.407 | -14.714 | 1.00 | 34.34 |
| ATOM | 453 | CA  | HIS A | 62 | 12.458 | 82.076 | -14.436 | 1.00 | 37.14 |
| ATOM | 454 | CB  | HIS A | 62 | 12.556 | 80.693 | -13.779 | 1.00 | 32.21 |
| ATOM | 455 | CG  | HIS A | 62 | 12.181 | 80.696 | -12.331 | 1.00 | 31.98 |
| ATOM | 456 | CD2 | HIS A | 62 | 11.234 | 80.007 | -11.652 | 1.00 | 29.94 |
| ATOM | 457 | ND1 | HIS A | 62 | 12.792 | 81.519 | -11.410 | 1.00 | 28.87 |
| ATOM | 458 | CE1 | HIS A | 62 | 12.234 | 81.344 | -10.228 | 1.00 | 28.92 |
| ATOM | 459 | NE2 | HIS A | 62 | 11.286 | 80.432 | -10.347 | 1.00 | 29.72 |
| ATOM | 460 | C   | HIS A | 62 | 13.437 | 82.193 | -15.599 | 1.00 | 41.35 |
| ATOM | 461 | O   | HIS A | 62 | 14.604 | 82.546 | -15.405 | 1.00 | 40.97 |
| ATOM | 462 | N   | MET A | 63 | 12.968 | 81.941 | -16.809 | 1.00 | 43.02 |
| ATOM | 463 | CA  | MET A | 63 | 13.867 | 82.018 | -17.941 | 1.00 | 45.13 |
| ATOM | 464 | CB  | MET A | 63 | 13.396 | 81.102 | -19.070 | 1.00 | 51.35 |
| ATOM | 465 | CG  | MET A | 63 | 13.180 | 79.653 | -18.631 | 1.00 | 63.00 |
| ATOM | 466 | SD  | MET A | 63 | 14.560 | 78.941 | -17.665 | 1.00 | 73.59 |
| ATOM | 467 | CE  | MET A | 63 | 15.229 | 77.786 | -18.858 | 1.00 | 73.56 |
| ATOM | 468 | C   | MET A | 63 | 14.052 | 83.438 | -18.445 | 1.00 | 44.26 |
| ATOM | 469 | O   | MET A | 63 | 15.126 | 83.781 | -18.927 | 1.00 | 50.29 |
| ATOM | 470 | N   | SER A | 64 | 13.041 | 84.283 | -18.287 | 1.00 | 39.05 |
| ATOM | 471 | CA  | SER A | 64 | 13.133 | 85.648 | -18.782 | 1.00 | 36.67 |
| ATOM | 472 | CB  | SER A | 64 | 11.798 | 86.062 | -19.386 | 1.00 | 37.55 |
| ATOM | 473 | OG  | SER A | 64 | 10.763 | 86.008 | -18.428 | 1.00 | 43.44 |
| ATOM | 474 | C   | SER A | 64 | 13.611 | 86.739 | -17.837 | 1.00 | 39.95 |
| ATOM | 475 | O   | SER A | 64 | 14.019 | 87.806 | -18.296 | 1.00 | 45.98 |
| ATOM | 476 | N   | ILE A | 65 | 13.486 | 86.531 | -16.530 | 1.00 | 41.66 |
| ATOM | 477 | CA  | ILE A | 65 | 13.914 | 87.547 | -15.568 | 1.00 | 37.23 |
| ATOM | 478 | CB  | ILE A | 65 | 13.477 | 87.209 | -14.108 | 1.00 | 35.14 |
| ATOM | 479 | CG2 | ILE A | 65 | 14.228 | 86.007 | -13.559 | 1.00 | 26.54 |
| ATOM | 480 | CG1 | ILE A | 65 | 13.725 | 88.412 | -13.207 | 1.00 | 31.65 |
| ATOM | 481 | CD1 | ILE A | 65 | 12.960 | 88.365 | -11.914 | 1.00 | 37.39 |
| ATOM | 482 | C   | ILE A | 65 | 15.420 | 87.732 | -15.672 | 1.00 | 38.75 |
| ATOM | 483 | O   | ILE A | 65 | 16.165 | 86.757 | -15.710 | 1.00 | 43.09 |
| ATOM | 484 | N   | THR A | 66 | 15.857 | 88.980 | -15.785 | 1.00 | 38.80 |
| ATOM | 485 | CA  | THR A | 66 | 17.278 | 89.281 | -15.924 | 1.00 | 39.81 |
| ATOM | 486 | CB  | THR A | 66 | 17.486 | 90.544 | -16.776 | 1.00 | 40.56 |
| ATOM | 487 | OG1 | THR A | 66 | 16.886 | 91.663 | -16.113 | 1.00 | 47.40 |
| ATOM | 488 | CG2 | THR A | 66 | 16.854 | 90.371 | -18.139 | 1.00 | 41.17 |
| ATOM | 489 | C   | THR A | 66 | 17.948 | 89.502 | -14.580 | 1.00 | 39.84 |
| ATOM | 490 | O   | THR A | 66 | 17.291 | 89.829 | -13.597 | 1.00 | 46.85 |
| ATOM | 491 | N   | PRO A | 67 | 19.279 | 89.365 | -14.524 | 1.00 | 40.14 |
| ATOM | 492 | CD  | PRO A | 67 | 20.152 | 88.850 | -15.590 | 1.00 | 39.50 |
| ATOM | 493 | CA  | PRO A | 67 | 20.037 | 89.557 | -13.281 | 1.00 | 39.40 |
| ATOM | 494 | CB  | PRO A | 67 | 21.482 | 89.273 | -13.709 | 1.00 | 39.30 |
| ATOM | 495 | CG  | PRO A | 67 | 21.459 | 89.446 | -15.212 | 1.00 | 40.61 |
| ATOM | 496 | C   | PRO A | 67 | 19.884 | 90.924 | -12.604 | 1.00 | 39.27 |
| ATOM | 497 | O   | PRO A | 67 | 19.934 | 91.012 | -11.378 | 1.00 | 42.45 |
| ATOM | 498 | N   | GLU A | 68 | 19.704 | 91.986 | -13.387 | 1.00 | 37.98 |
| ATOM | 499 | CA  | GLU A | 68 | 19.528 | 93.316 | -12.811 | 1.00 | 36.08 |
| ATOM | 500 | CB  | GLU A | 68 | 19.598 | 94.425 | -13.865 | 1.00 | 44.41 |
| ATOM | 501 | CG  | GLU A | 68 | 20.830 | 94.408 | -14.745 | 1.00 | 56.01 |
| ATOM | 502 | CD  | GLU A | 68 | 20.701 | 93.426 | -15.897 | 1.00 | 62.86 |
| ATOM | 503 | OE1 | GLU A | 68 | 19.776 | 93.599 | -16.727 | 1.00 | 65.53 |
| ATOM | 504 | OE2 | GLU A | 68 | 21.519 | 92.480 | -15.972 | 1.00 | 66.08 |
| ATOM | 505 | C   | GLU A | 68 | 18.166 | 93.349 | -12.157 | 1.00 | 32.92 |
| ATOM | 506 | O   | GLU A | 68 | 17.968 | 94.037 | -11.158 | 1.00 | 37.34 |
| ATOM | 507 | N   | GLU A | 69 | 17.217 | 92.633 | -12.747 | 1.00 | 28.56 |

|      |     |     |       |    |        |        |         |      |       |
|------|-----|-----|-------|----|--------|--------|---------|------|-------|
| ATOM | 508 | CA  | GLU A | 69 | 15.877 | 92.560 | -12.193 | 1.00 | 26.48 |
| ATOM | 509 | CB  | GLU A | 69 | 14.927 | 91.889 | -13.170 | 1.00 | 26.48 |
| ATOM | 510 | CG  | GLU A | 69 | 14.696 | 92.647 | -14.438 | 1.00 | 31.14 |
| ATOM | 511 | CD  | GLU A | 69 | 13.480 | 92.145 | -15.147 | 1.00 | 36.47 |
| ATOM | 512 | OE1 | GLU A | 69 | 12.386 | 92.682 | -14.875 | 1.00 | 41.34 |
| ATOM | 513 | OE2 | GLU A | 69 | 13.612 | 91.195 | -15.946 | 1.00 | 41.53 |
| ATOM | 514 | C   | GLU A | 69 | 15.925 | 91.749 | -10.900 | 1.00 | 26.61 |
| ATOM | 515 | O   | GLU A | 69 | 15.268 | 92.086 | -9.916  | 1.00 | 33.09 |
| ATOM | 516 | N   | LYS A | 70 | 16.703 | 90.672 | -10.902 | 1.00 | 23.31 |
| ATOM | 517 | CA  | LYS A | 70 | 16.830 | 89.844 | -9.719  | 1.00 | 18.07 |
| ATOM | 518 | CB  | LYS A | 70 | 17.730 | 88.655 | -10.000 | 1.00 | 16.10 |
| ATOM | 519 | CG  | LYS A | 70 | 17.125 | 87.693 | -10.978 | 1.00 | 16.50 |
| ATOM | 520 | CD  | LYS A | 70 | 18.081 | 86.602 | -11.323 | 1.00 | 19.40 |
| ATOM | 521 | CE  | LYS A | 70 | 17.421 | 85.611 | -12.243 | 1.00 | 23.23 |
| ATOM | 522 | NZ  | LYS A | 70 | 18.372 | 84.538 | -12.604 | 1.00 | 28.38 |
| ATOM | 523 | C   | LYS A | 70 | 17.397 | 90.685 | -8.596  | 1.00 | 22.66 |
| ATOM | 524 | O   | LYS A | 70 | 16.836 | 90.725 | -7.505  | 1.00 | 27.15 |
| ATOM | 525 | N   | TRP A | 71 | 18.461 | 91.424 | -8.891  | 1.00 | 21.96 |
| ATOM | 526 | CA  | TRP A | 71 | 19.101 | 92.274 | -7.897  | 1.00 | 22.52 |
| ATOM | 527 | CB  | TRP A | 71 | 20.321 | 92.982 | -8.494  | 1.00 | 19.42 |
| ATOM | 528 | CG  | TRP A | 71 | 21.037 | 93.865 | -7.506  | 1.00 | 20.03 |
| ATOM | 529 | CD2 | TRP A | 71 | 21.800 | 93.441 | -6.366  | 1.00 | 17.51 |
| ATOM | 530 | CE2 | TRP A | 71 | 22.293 | 94.604 | -5.736  | 1.00 | 15.91 |
| ATOM | 531 | CE3 | TRP A | 71 | 22.103 | 92.194 | -5.809  | 1.00 | 19.70 |
| ATOM | 532 | CD1 | TRP A | 71 | 21.104 | 95.230 | -7.524  | 1.00 | 18.18 |
| ATOM | 533 | NE1 | TRP A | 71 | 21.859 | 95.680 | -6.466  | 1.00 | 21.55 |
| ATOM | 534 | CZ2 | TRP A | 71 | 23.089 | 94.559 | -4.585  | 1.00 | 20.06 |
| ATOM | 535 | CZ3 | TRP A | 71 | 22.897 | 92.147 | -4.662  | 1.00 | 20.49 |
| ATOM | 536 | CH2 | TRP A | 71 | 23.373 | 93.324 | -4.061  | 1.00 | 20.53 |
| ATOM | 537 | C   | TRP A | 71 | 18.123 | 93.299 | -7.359  | 1.00 | 23.60 |
| ATOM | 538 | O   | TRP A | 71 | 18.089 | 93.584 | -6.155  | 1.00 | 24.12 |
| ATOM | 539 | N   | ASP A | 72 | 17.327 | 93.860 | -8.254  | 1.00 | 23.56 |
| ATOM | 540 | CA  | ASP A | 72 | 16.358 | 94.859 | 7.860   | 1.00 | 27.03 |
| ATOM | 541 | CB  | ASP A | 72 | 15.853 | 95.630 | -9.083  | 1.00 | 34.54 |
| ATOM | 542 | CG  | ASP A | 72 | 16.921 | 96.534 | -9.692  | 1.00 | 40.55 |
| ATOM | 543 | OD1 | ASP A | 72 | 18.116 | 96.375 | -9.363  | 1.00 | 47.37 |
| ATOM | 544 | OD2 | ASP A | 72 | 16.563 | 97.416 | -10.502 | 1.00 | 50.79 |
| ATOM | 545 | C   | ASP A | 72 | 15.208 | 94.309 | -7.032  | 1.00 | 26.53 |
| ATOM | 546 | O   | ASP A | 72 | 14.506 | 95.082 | -6.384  | 1.00 | 33.99 |
| ATOM | 547 | N   | LEU A | 73 | 15.055 | 92.989 | -6.999  | 1.00 | 23.44 |
| ATOM | 548 | CA  | LEU A | 73 | 13.998 | 92.353 | -6.224  | 1.00 | 19.61 |
| ATOM | 549 | CB  | LEU A | 73 | 13.219 | 91.372 | -7.091  | 1.00 | 20.50 |
| ATOM | 550 | CG  | LEU A | 73 | 12.333 | 91.920 | -8.201  | 1.00 | 20.73 |
| ATOM | 551 | CD1 | LEU A | 73 | 11.692 | 90.760 | -8.945  | 1.00 | 10.89 |
| ATOM | 552 | CD2 | LEU A | 73 | 11.280 | 92.830 | -7.601  | 1.00 | 14.36 |
| ATOM | 553 | C   | LEU A | 73 | 14.558 | 91.581 | -5.049  | 1.00 | 19.51 |
| ATOM | 554 | O   | LEU A | 73 | 13.811 | 91.098 | -4.212  | 1.00 | 22.35 |
| ATOM | 555 | N   | ALA A | 74 | 15.871 | 91.415 | -5.019  | 1.00 | 20.26 |
| ATOM | 556 | CA  | ALA A | 74 | 16.535 | 90.656 | -3.965  | 1.00 | 18.26 |
| ATOM | 557 | CB  | ALA A | 74 | 18.046 | 90.726 | -4.146  | 1.00 | 17.07 |
| ATOM | 558 | C   | ALA A | 74 | 16.163 | 91.106 | -2.569  | 1.00 | 19.57 |
| ATOM | 559 | O   | ALA A | 74 | 15.917 | 92.285 | -2.344  | 1.00 | 17.06 |
| ATOM | 560 | N   | ILE A | 75 | 16.115 | 90.157 | -1.637  | 1.00 | 21.97 |
| ATOM | 561 | CA  | ILE A | 75 | 15.811 | 90.457 | -0.239  | 1.00 | 18.37 |
| ATOM | 562 | CB  | ILE A | 75 | 15.337 | 89.202 | 0.514   | 1.00 | 15.88 |
| ATOM | 563 | CG2 | ILE A | 75 | 14.056 | 88.700 | -0.073  | 1.00 | 15.90 |
| ATOM | 564 | CG1 | ILE A | 75 | 16.380 | 88.096 | 0.422   | 1.00 | 17.42 |
| ATOM | 565 | CD1 | ILE A | 75 | 16.178 | 86.992 | 1.424   | 1.00 | 20.14 |
| ATOM | 566 | C   | ILE A | 75 | 17.051 | 91.063 | 0.453   | 1.00 | 22.26 |
| ATOM | 567 | O   | ILE A | 75 | 18.155 | 91.028 | -0.093  | 1.00 | 24.15 |
| ATOM | 568 | N   | ARG A | 76 | 16.866 | 91.598 | 1.656   | 1.00 | 23.62 |
| ATOM | 569 | CA  | ARG A | 76 | 17.934 | 92.244 | 2.423   | 1.00 | 22.51 |
| ATOM | 570 | CB  | ARG A | 76 | 17.382 | 92.683 | 3.776   | 1.00 | 25.41 |
| ATOM | 571 | CG  | ARG A | 76 | 18.277 | 93.622 | 4.540   | 1.00 | 30.98 |
| ATOM | 572 | CD  | ARG A | 76 | 17.650 | 93.958 | 5.878   | 1.00 | 39.61 |
| ATOM | 573 | NE  | ARG A | 76 | 17.503 | 92.780 | 6.731   | 1.00 | 43.97 |
| ATOM | 574 | CZ  | ARG A | 76 | 16.615 | 92.675 | 7.719   | 1.00 | 46.12 |
| ATOM | 575 | NH1 | ARG A | 76 | 15.786 | 93.678 | 7.995   | 1.00 | 44.59 |
| ATOM | 576 | NH2 | ARG A | 76 | 16.533 | 91.550 | 8.417   | 1.00 | 44.99 |
| ATOM | 577 | C   | ARG A | 76 | 19.199 | 91.410 | 2.622   | 1.00 | 20.90 |
| ATOM | 578 | O   | ARG A | 76 | 20.303 | 91.939 | 2.667   | 1.00 | 21.19 |
| ATOM | 579 | N   | ALA A | 77 | 19.037 | 90.105 | 2.773   | 1.00 | 22.00 |
| ATOM | 580 | CA  | ALA A | 77 | 20.175 | 89.219 | 2.962   | 1.00 | 20.40 |

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|      |     |     |       |    |        |         |        |      |       |
|------|-----|-----|-------|----|--------|---------|--------|------|-------|
| ATOM | 581 | CB  | ALA A | 77 | 19.706 | 87.798  | 3.239  | 1.00 | 16.39 |
| ATOM | 582 | C   | ALA A | 77 | 21.127 | 89.245  | 1.770  | 1.00 | 24.32 |
| ATOM | 583 | O   | ALA A | 77 | 22.275 | 88.824  | 1.889  | 1.00 | 29.02 |
| ATOM | 584 | N   | TYR A | 78 | 20.643 | 89.704  | 0.618  | 1.00 | 25.15 |
| ATOM | 585 | CA  | TYR A | 78 | 21.471 | 89.795  | -0.587 | 1.00 | 19.05 |
| ATOM | 586 | CB  | TYR A | 78 | 20.810 | 89.103  | -1.764 | 1.00 | 16.11 |
| ATOM | 587 | CG  | TYR A | 78 | 20.748 | 87.618  | -1.613 | 1.00 | 16.70 |
| ATOM | 588 | CD1 | TYR A | 78 | 19.611 | 87.000  | -1.114 | 1.00 | 15.71 |
| ATOM | 589 | CE1 | TYR A | 78 | 19.542 | 85.626  | -1.006 | 1.00 | 14.79 |
| ATOM | 590 | CD2 | TYR A | 78 | 21.821 | 86.823  | -1.987 | 1.00 | 17.98 |
| ATOM | 591 | CE2 | TYR A | 78 | 21.762 | 85.458  | -1.886 | 1.00 | 15.81 |
| ATOM | 592 | CZ  | TYR A | 78 | 20.624 | 84.864  | -1.394 | 1.00 | 19.26 |
| ATOM | 593 | OH  | TYR A | 78 | 20.563 | 83.495  | -1.336 | 1.00 | 27.92 |
| ATOM | 594 | C   | TYR A | 78 | 21.735 | 91.233  | -0.952 | 1.00 | 18.90 |
| ATOM | 595 | O   | TYR A | 78 | 22.874 | 91.609  | -1.178 | 1.00 | 24.83 |
| ATOM | 596 | N   | ASN A | 79 | 20.672 | 92.025  | -1.046 | 1.00 | 20.12 |
| ATOM | 597 | CA  | ASN A | 79 | 20.778 | 93.442  | -1.396 | 1.00 | 23.74 |
| ATOM | 598 | CB  | ASN A | 79 | 19.767 | 93.794  | -2.491 | 1.00 | 21.09 |
| ATOM | 599 | CG  | ASN A | 79 | 19.985 | 95.173  | -3.071 | 1.00 | 20.38 |
| ATOM | 600 | OD1 | ASN A | 79 | 20.558 | 96.049  | -2.437 | 1.00 | 24.59 |
| ATOM | 601 | ND2 | ASN A | 79 | 19.511 | 95.378  | -4.283 | 1.00 | 17.81 |
| ATOM | 602 | C   | ASN A | 79 | 20.563 | 94.310  | -0.161 | 1.00 | 26.18 |
| ATOM | 603 | O   | ASN A | 79 | 19.442 | 94.645  | 0.206  | 1.00 | 28.37 |
| ATOM | 604 | N   | LYS A | 80 | 21.668 | 94.695  | 0.452  | 1.00 | 28.39 |
| ATOM | 605 | CA  | LYS A | 80 | 21.693 | 95.496  | 1.663  | 1.00 | 28.15 |
| ATOM | 606 | CB  | LYS A | 80 | 23.145 | 95.869  | 1.926  | 1.00 | 30.31 |
| ATOM | 607 | CG  | LYS A | 80 | 23.434 | 96.446  | 3.270  | 1.00 | 41.68 |
| ATOM | 608 | CD  | LYS A | 80 | 24.934 | 96.530  | 3.472  | 1.00 | 49.85 |
| ATOM | 609 | CE  | LYS A | 80 | 25.290 | 97.287  | 4.739  | 1.00 | 56.09 |
| ATOM | 610 | NZ  | LYS A | 80 | 26.764 | 97.261  | 4.971  | 1.00 | 59.86 |
| ATOM | 611 | C   | LYS A | 80 | 20.805 | 96.741  | 1.640  | 1.00 | 28.30 |
| ATOM | 612 | O   | LYS A | 80 | 20.388 | 97.234  | 2.679  | 1.00 | 31.85 |
| ATOM | 613 | N   | GLU A | 81 | 20.444 | 97.183  | 0.448  | 1.00 | 27.68 |
| ATOM | 614 | CA  | GLU A | 81 | 19.631 | 98.377  | 0.245  | 1.00 | 27.82 |
| ATOM | 615 | CB  | GLU A | 81 | 19.700 | 98.738  | -1.245 | 1.00 | 26.85 |
| ATOM | 616 | CG  | GLU A | 81 | 18.936 | 99.974  | -1.667 | 1.00 | 25.54 |
| ATOM | 617 | CD  | GLU A | 81 | 18.843 | 100.115 | -3.173 | 1.00 | 27.23 |
| ATOM | 618 | OE1 | GLU A | 81 | 18.424 | 101.187 | -3.645 | 1.00 | 30.11 |
| ATOM | 619 | OE2 | GLU A | 81 | 19.177 | 99.153  | -3.892 | 1.00 | 35.72 |
| ATOM | 620 | C   | GLU A | 81 | 18.163 | 98.261  | 0.685  | 1.00 | 28.54 |
| ATOM | 621 | O   | GLU A | 81 | 17.592 | 99.190  | 1.260  | 1.00 | 32.85 |
| ATOM | 622 | N   | HIS A | 82 | 17.544 | 97.125  | 0.400  | 1.00 | 28.51 |
| ATOM | 623 | CA  | HIS A | 82 | 16.145 | 96.919  | 0.736  | 1.00 | 26.34 |
| ATOM | 624 | CB  | HIS A | 82 | 15.547 | 95.839  | -0.148 | 1.00 | 23.16 |
| ATOM | 625 | CG  | HIS A | 82 | 15.992 | 95.898  | -1.569 | 1.00 | 20.08 |
| ATOM | 626 | CD2 | HIS A | 82 | 16.006 | 96.906  | -2.467 | 1.00 | 14.88 |
| ATOM | 627 | ND1 | HIS A | 82 | 16.428 | 94.781  | -2.241 | 1.00 | 21.04 |
| ATOM | 628 | CE1 | HIS A | 82 | 16.684 | 95.094  | -3.493 | 1.00 | 20.58 |
| ATOM | 629 | NE2 | HIS A | 82 | 16.433 | 96.382  | -3.661 | 1.00 | 16.40 |
| ATOM | 630 | C   | HIS A | 82 | 15.992 | 96.461  | 2.168  | 1.00 | 29.32 |
| ATOM | 631 | O   | HIS A | 82 | 15.653 | 95.302  | 2.415  | 1.00 | 29.56 |
| ATOM | 632 | N   | GLN A | 83 | 16.193 | 97.366  | 3.113  | 1.00 | 32.90 |
| ATOM | 633 | CA  | GLN A | 83 | 16.084 | 97.006  | 4.517  | 1.00 | 36.06 |
| ATOM | 634 | CB  | GLN A | 83 | 16.438 | 98.194  | 5.406  | 1.00 | 42.46 |
| ATOM | 635 | CG  | GLN A | 83 | 17.942 | 98.406  | 5.566  | 1.00 | 54.39 |
| ATOM | 636 | CD  | GLN A | 83 | 18.637 | 97.224  | 6.227  | 1.00 | 60.00 |
| ATOM | 637 | OE1 | GLN A | 83 | 18.366 | 96.899  | 7.386  | 1.00 | 66.86 |
| ATOM | 638 | NE2 | GLN A | 83 | 19.934 | 96.572  | 5.492  | 1.00 | 60.20 |
| ATOM | 639 | C   | GLN A | 83 | 14.746 | 96.418  | 4.932  | 1.00 | 34.12 |
| ATOM | 640 | O   | GLN A | 83 | 14.689 | 95.623  | 5.856  | 1.00 | 36.75 |
| ATOM | 641 | N   | ASP A | 84 | 13.684 | 96.755  | 4.215  | 1.00 | 35.26 |
| ATOM | 642 | CA  | ASP A | 84 | 12.353 | 96.260  | 4.546  | 1.00 | 35.02 |
| ATOM | 643 | CB  | ASP A | 84 | 11.293 | 97.298  | 4.158  | 1.00 | 47.91 |
| ATOM | 644 | CG  | ASP A | 84 | 11.437 | 98.611  | 4.925  | 1.00 | 61.72 |
| ATOM | 645 | OD1 | ASP A | 84 | 11.115 | 99.673  | 4.344  | 1.00 | 68.07 |
| ATOM | 646 | OD2 | ASP A | 84 | 11.863 | 98.587  | 6.104  | 1.00 | 69.22 |
| ATOM | 647 | C   | ASP A | 84 | 11.987 | 94.912  | 3.931  | 1.00 | 30.42 |
| ATOM | 648 | O   | ASP A | 84 | 10.890 | 94.402  | 4.158  | 1.00 | 31.96 |
| ATOM | 649 | N   | GLN A | 85 | 12.881 | 94.331  | 3.146  | 1.00 | 23.30 |
| ATOM | 650 | CA  | GLN A | 85 | 12.571 | 93.058  | 2.537  | 1.00 | 20.72 |
| ATOM | 651 | CB  | GLN A | 85 | 12.946 | 93.059  | 1.068  | 1.00 | 20.88 |
| ATOM | 652 | CG  | GLN A | 85 | 12.181 | 94.019  | 0.236  | 1.00 | 23.30 |
| ATOM | 653 | CD  | GLN A | 85 | 12.434 | 93.811  | -1.235 | 1.00 | 32.07 |

|      |     |     |       |    |        |        |         |      |       |
|------|-----|-----|-------|----|--------|--------|---------|------|-------|
| ATOM | 654 | OE1 | GLN A | 85 | 12.670 | 94.762 | -1.982  | 1.00 | 41.97 |
| ATOM | 655 | NE2 | GLN A | 85 | 12.378 | 92.565 | -1.666  | 1.00 | 31.81 |
| ATOM | 656 | C   | GLN A | 85 | 13.286 | 91.930 | 3.242   | 1.00 | 22.01 |
| ATOM | 657 | O   | GLN A | 85 | 14.485 | 91.736 | 3.061   | 1.00 | 25.61 |
| ATOM | 658 | N   | VAL A | 86 | 12.551 | 91.171 | 4.038   | 1.00 | 21.04 |
| ATOM | 659 | CA  | VAL A | 86 | 13.151 | 90.063 | 4.758   | 1.00 | 20.72 |
| ATOM | 660 | CB  | VAL A | 86 | 12.835 | 90.127 | 6.271   | 1.00 | 23.91 |
| ATOM | 661 | CG1 | VAL A | 86 | 13.522 | 88.996 | 6.993   | 1.00 | 24.41 |
| ATOM | 662 | CG2 | VAL A | 86 | 13.272 | 91.445 | 6.856   | 1.00 | 24.17 |
| ATOM | 663 | C   | VAL A | 86 | 12.717 | 88.713 | 4.204   | 1.00 | 20.58 |
| ATOM | 664 | O   | VAL A | 86 | 13.554 | 87.851 | 3.990   | 1.00 | 29.31 |
| ATOM | 665 | N   | ARG A | 87 | 11.417 | 88.530 | 3.990   | 1.00 | 18.86 |
| ATOM | 666 | CA  | ARG A | 87 | 10.875 | 87.270 | 3.467   | 1.00 | 18.95 |
| ATOM | 667 | CB  | ARG A | 87 | 9.560  | 86.885 | 4.153   | 1.00 | 21.46 |
| ATOM | 668 | CG  | ARG A | 87 | 9.591  | 86.566 | 5.630   | 1.00 | 24.00 |
| ATOM | 669 | CD  | ARG A | 87 | 8.153  | 86.365 | 6.142   | 1.00 | 23.85 |
| ATOM | 670 | NE  | ARG A | 87 | 7.549  | 85.127 | 5.647   | 1.00 | 26.86 |
| ATOM | 671 | CZ  | ARG A | 87 | 6.252  | 84.833 | 5.742   | 1.00 | 24.59 |
| ATOM | 672 | NH1 | ARG A | 87 | 5.412  | 85.691 | 6.300   | 1.00 | 22.47 |
| ATOM | 673 | NH2 | ARG A | 87 | 5.803  | 83.654 | 5.333   | 1.00 | 22.94 |
| ATOM | 674 | C   | ARG A | 87 | 10.548 | 87.409 | 1.989   | 1.00 | 17.44 |
| ATOM | 675 | O   | ARG A | 87 | 10.947 | 86.591 | 1.181   | 1.00 | 20.34 |
| ATOM | 676 | N   | ALA A | 88 | 9.803  | 88.456 | 1.657   | 1.00 | 14.27 |
| ATOM | 677 | CA  | ALA A | 88 | 9.353  | 88.708 | 0.296   | 1.00 | 15.50 |
| ATOM | 678 | CB  | ALA A | 88 | 8.154  | 89.637 | 0.307   | 1.00 | 11.55 |
| ATOM | 679 | C   | ALA A | 88 | 10.413 | 89.247 | -0.630  | 1.00 | 18.22 |
| ATOM | 680 | O   | ALA A | 88 | 11.122 | 90.190 | -0.284  | 1.00 | 24.16 |
| ATOM | 681 | N   | GLY A | 89 | 10.461 | 88.688 | -1.837  | 1.00 | 18.31 |
| ATOM | 682 | CA  | GLY A | 89 | 11.437 | 89.103 | -2.825  | 1.00 | 18.37 |
| ATOM | 683 | C   | GLY A | 89 | 12.221 | 87.946 | -3.422  | 1.00 | 21.93 |
| ATOM | 684 | O   | GLY A | 89 | 11.853 | 86.773 | -3.262  | 1.00 | 23.18 |
| ATOM | 685 | N   | TYR A | 90 | 13.315 | 88.286 | -4.103  | 1.00 | 21.46 |
| ATOM | 686 | CA  | TYR A | 90 | 14.178 | 87.314 | -4.767  | 1.00 | 17.61 |
| ATOM | 687 | CB  | TYR A | 90 | 14.701 | 87.909 | -6.098  | 1.00 | 14.11 |
| ATOM | 688 | CG  | TYR A | 90 | 14.847 | 86.895 | -7.215  | 1.00 | 15.32 |
| ATOM | 689 | CD1 | TYR A | 90 | 13.827 | 86.705 | -8.142  | 1.00 | 15.35 |
| ATOM | 690 | CE1 | TYR A | 90 | 13.900 | 85.686 | -9.100  | 1.00 | 17.27 |
| ATOM | 691 | CD2 | TYR A | 90 | 15.963 | 86.050 | -7.283  | 1.00 | 17.90 |
| ATOM | 692 | CE2 | TYR A | 90 | 16.047 | 85.031 | -8.236  | 1.00 | 18.10 |
| ATOM | 693 | CZ  | TYR A | 90 | 15.010 | 84.855 | -9.136  | 1.00 | 18.33 |
| ATOM | 694 | OH  | TYR A | 90 | 15.056 | 83.829 | -10.056 | 1.00 | 29.46 |
| ATOM | 695 | C   | TYR A | 90 | 15.344 | 86.861 | -3.881  | 1.00 | 18.14 |
| ATOM | 696 | O   | TYR A | 90 | 15.877 | 87.636 | -3.089  | 1.00 | 19.67 |
| ATOM | 697 | N   | TYR A | 91 | 15.713 | 85.592 | -4.013  | 1.00 | 20.08 |
| ATOM | 698 | CA  | TYR A | 91 | 16.819 | 84.976 | -3.277  | 1.00 | 20.39 |
| ATOM | 699 | CB  | TYR A | 91 | 16.354 | 83.713 | -2.542  | 1.00 | 20.44 |
| ATOM | 700 | CG  | TYR A | 91 | 15.353 | 83.965 | -1.432  | 1.00 | 20.34 |
| ATOM | 701 | CD1 | TYR A | 91 | 14.116 | 84.566 | -1.693  | 1.00 | 21.65 |
| ATOM | 702 | CE1 | TYR A | 91 | 13.211 | 84.819 | -0.677  | 1.00 | 16.23 |
| ATOM | 703 | CD2 | TYR A | 91 | 15.651 | 83.622 | -0.120  | 1.00 | 18.42 |
| ATOM | 704 | CE2 | TYR A | 91 | 14.753 | 83.867 | 0.898   | 1.00 | 20.40 |
| ATOM | 705 | CZ  | TYR A | 91 | 13.536 | 84.468 | 0.615   | 1.00 | 22.22 |
| ATOM | 706 | OH  | TYR A | 91 | 12.651 | 84.705 | 1.639   | 1.00 | 21.37 |
| ATOM | 707 | C   | TYR A | 91 | 17.819 | 84.603 | -4.362  | 1.00 | 23.73 |
| ATOM | 708 | O   | TYR A | 91 | 17.583 | 83.687 | -5.154  | 1.00 | 24.20 |
| ATOM | 709 | N   | LEU A | 92 | 18.894 | 85.374 | -4.451  | 1.00 | 28.01 |
| ATOM | 710 | CA  | LEU A | 92 | 19.909 | 85.160 | -5.476  | 1.00 | 24.96 |
| ATOM | 711 | CB  | LEU A | 92 | 20.857 | 86.362 | -5.534  | 1.00 | 24.17 |
| ATOM | 712 | CG  | LEU A | 92 | 20.258 | 87.756 | -5.635  | 1.00 | 19.59 |
| ATOM | 713 | CD1 | LEU A | 92 | 21.353 | 88.782 | -5.696  | 1.00 | 23.44 |
| ATOM | 714 | CD2 | LEU A | 92 | 19.406 | 87.837 | -6.850  | 1.00 | 22.64 |
| ATOM | 715 | C   | LEU A | 92 | 20.749 | 83.910 | -5.283  | 1.00 | 25.80 |
| ATOM | 716 | O   | LEU A | 92 | 20.879 | 83.382 | -4.174  | 1.00 | 25.07 |
| ATOM | 717 | N   | SER A | 93 | 21.310 | 83.440 | -6.387  | 1.00 | 26.00 |
| ATOM | 718 | CA  | SER A | 93 | 22.210 | 82.307 | -6.358  | 1.00 | 27.05 |
| ATOM | 719 | CB  | SER A | 93 | 22.218 | 81.584 | -7.703  | 1.00 | 24.34 |
| ATOM | 720 | OG  | SER A | 93 | 22.434 | 82.479 | -8.776  | 1.00 | 26.84 |
| ATOM | 721 | C   | SER A | 93 | 23.569 | 82.942 | -6.087  | 1.00 | 27.46 |
| ATOM | 722 | O   | SER A | 93 | 23.776 | 84.125 | -6.348  | 1.00 | 26.92 |
| ATOM | 723 | N   | ILE A | 94 | 24.487 | 82.178 | -5.530  | 1.00 | 29.65 |
| ATOM | 724 | CA  | ILE A | 94 | 25.797 | 82.716 | -5.234  | 1.00 | 31.96 |
| ATOM | 725 | CB  | ILE A | 94 | 26.106 | 82.624 | -3.740  | 1.00 | 33.15 |
| ATOM | 726 | CG2 | ILE A | 94 | 27.467 | 83.228 | -3.456  | 1.00 | 29.48 |

|      |     |     |       |     |        |        |         |      |       |
|------|-----|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 727 | CG1 | ILE A | 94  | 25.025 | 83.358 | -2.946  | 1.00 | 33.35 |
| ATOM | 728 | CD1 | ILE A | 94  | 25.093 | 83.120 | -1.463  | 1.00 | 36.58 |
| ATOM | 729 | C   | ILE A | 94  | 26.753 | 81.863 | -6.027  | 1.00 | 34.38 |
| ATOM | 730 | O   | ILE A | 94  | 26.946 | 80.691 | -5.717  | 1.00 | 36.74 |
| ATOM | 731 | N   | PRO A | 95  | 27.339 | 82.423 | -7.080  | 1.00 | 38.50 |
| ATOM | 732 | CD  | PRO A | 95  | 27.368 | 83.872 | -7.350  | 1.00 | 40.61 |
| ATOM | 733 | CA  | PRO A | 95  | 28.283 | 81.724 | -7.947  | 1.00 | 40.90 |
| ATOM | 734 | CB  | PRO A | 95  | 28.917 | 82.854 | -8.745  | 1.00 | 45.71 |
| ATOM | 735 | CG  | PRO A | 95  | 28.765 | 84.049 | -7.829  | 1.00 | 45.59 |
| ATOM | 736 | C   | PRO A | 95  | 29.309 | 80.929 | -7.159  | 1.00 | 39.51 |
| ATOM | 737 | O   | PRO A | 95  | 30.004 | 81.477 | -6.310  | 1.00 | 42.47 |
| ATOM | 738 | N   | GLY A | 96  | 29.327 | 79.625 | -7.391  | 1.00 | 38.51 |
| ATOM | 739 | CA  | GLY A | 96  | 30.259 | 78.752 | -6.713  | 1.00 | 35.63 |
| ATOM | 740 | C   | GLY A | 96  | 29.740 | 78.161 | -5.424  | 1.00 | 37.97 |
| ATOM | 741 | O   | GLY A | 96  | 30.126 | 77.062 | -5.047  | 1.00 | 39.52 |
| ATOM | 742 | N   | LYS A | 97  | 28.812 | 78.849 | -4.777  | 1.00 | 35.33 |
| ATOM | 743 | CA  | LYS A | 97  | 28.318 | 78.365 | -3.504  | 1.00 | 34.40 |
| ATOM | 744 | CB  | LYS A | 97  | 28.555 | 79.419 | -2.435  | 1.00 | 42.78 |
| ATOM | 745 | CG  | LYS A | 97  | 29.982 | 79.900 | -2.352  | 1.00 | 54.46 |
| ATOM | 746 | CD  | LYS A | 97  | 30.041 | 81.101 | -1.428  | 1.00 | 65.72 |
| ATOM | 747 | CE  | LYS A | 97  | 31.450 | 81.651 | -1.284  | 1.00 | 73.04 |
| ATOM | 748 | NZ  | LYS A | 97  | 31.498 | 82.894 | -0.447  | 1.00 | 78.91 |
| ATOM | 749 | C   | LYS A | 97  | 26.857 | 77.959 | -3.450  | 1.00 | 32.83 |
| ATOM | 750 | O   | LYS A | 97  | 26.501 | 77.068 | -2.683  | 1.00 | 34.44 |
| ATOM | 751 | N   | LYS A | 98  | 26.008 | 78.603 | -4.243  | 1.00 | 26.62 |
| ATOM | 752 | CA  | LYS A | 98  | 24.574 | 78.319 | -4.215  | 1.00 | 22.39 |
| ATOM | 753 | CB  | LYS A | 98  | 23.876 | 79.351 | -3.319  | 1.00 | 23.74 |
| ATOM | 754 | CG  | LYS A | 98  | 22.362 | 79.269 | -3.276  | 1.00 | 22.19 |
| ATOM | 755 | CD  | LYS A | 98  | 21.766 | 80.300 | -2.335  | 1.00 | 22.81 |
| ATOM | 756 | CE  | LYS A | 98  | 20.251 | 80.160 | -2.241  | 1.00 | 22.30 |
| ATOM | 757 | NZ  | LYS A | 98  | 19.547 | 80.977 | -3.253  | 1.00 | 21.47 |
| ATOM | 758 | C   | LYS A | 98  | 23.990 | 78.346 | -5.614  | 1.00 | 21.39 |
| ATOM | 759 | O   | LYS A | 98  | 24.076 | 79.355 | -6.301  | 1.00 | 23.12 |
| ATOM | 760 | N   | ALA A | 99  | 23.427 | 77.225 | -6.044  | 1.00 | 21.69 |
| ATOM | 761 | CA  | ALA A | 99  | 22.819 | 77.132 | -7.369  | 1.00 | 23.49 |
| ATOM | 762 | CB  | ALA A | 99  | 23.126 | 75.756 | -7.983  | 1.00 | 21.77 |
| ATOM | 763 | C   | ALA A | 99  | 21.301 | 77.449 | -7.439  | 1.00 | 22.78 |
| ATOM | 764 | O   | ALA A | 99  | 20.834 | 78.065 | -8.399  | 1.00 | 25.07 |
| ATOM | 765 | N   | VAL A | 100 | 20.547 | 77.040 | -6.420  | 1.00 | 20.36 |
| ATOM | 766 | CA  | VAL A | 100 | 19.106 | 77.274 | -6.388  | 1.00 | 17.58 |
| ATOM | 767 | CB  | VAL A | 100 | 18.462 | 76.528 | -5.196  | 1.00 | 16.99 |
| ATOM | 768 | CG1 | VAL A | 100 | 16.971 | 76.786 | -5.130  | 1.00 | 14.03 |
| ATOM | 769 | CG2 | VAL A | 100 | 18.722 | 75.044 | -5.313  | 1.00 | 15.21 |
| ATOM | 770 | C   | VAL A | 100 | 18.797 | 78.764 | -6.277  | 1.00 | 20.86 |
| ATOM | 771 | O   | VAL A | 100 | 19.574 | 79.506 | -5.697  | 1.00 | 25.82 |
| ATOM | 772 | N   | GLU A | 101 | 17.696 | 79.201 | -6.885  | 1.00 | 20.04 |
| ATOM | 773 | CA  | GLU A | 101 | 17.236 | 80.595 | -6.829  | 1.00 | 17.64 |
| ATOM | 774 | CB  | GLU A | 101 | 17.352 | 81.316 | -8.185  | 1.00 | 22.33 |
| ATOM | 775 | CG  | GLU A | 101 | 18.682 | 81.355 | -8.862  | 1.00 | 27.61 |
| ATOM | 776 | CD  | GLU A | 101 | 18.654 | 82.264 | -10.048 | 1.00 | 28.27 |
| ATOM | 777 | OE1 | GLU A | 101 | 19.711 | 82.803 | -10.393 | 1.00 | 35.84 |
| ATOM | 778 | OE2 | GLU A | 101 | 17.591 | 82.440 | -10.656 | 1.00 | 33.44 |
| ATOM | 779 | C   | GLU A | 101 | 15.734 | 80.502 | -6.561  | 1.00 | 18.04 |
| ATOM | 780 | O   | GLU A | 101 | 15.085 | 79.542 | -6.977  | 1.00 | 20.27 |
| ATOM | 781 | N   | SER A | 102 | 15.151 | 81.543 | -5.989  | 1.00 | 15.18 |
| ATOM | 782 | CA  | SER A | 102 | 13.727 | 81.512 | -5.749  | 1.00 | 14.63 |
| ATOM | 783 | CB  | SER A | 102 | 13.372 | 80.575 | -4.599  | 1.00 | 16.17 |
| ATOM | 784 | OG  | SER A | 102 | 14.095 | 80.881 | -3.441  | 1.00 | 19.01 |
| ATOM | 785 | C   | SER A | 102 | 13.172 | 82.883 | -5.512  | 1.00 | 14.90 |
| ATOM | 786 | O   | SER A | 102 | 13.919 | 83.805 | -5.226  | 1.00 | 16.69 |
| ATOM | 787 | N   | PHE A | 103 | 11.871 | 83.018 | -5.753  | 1.00 | 16.08 |
| ATOM | 788 | CA  | PHE A | 103 | 11.135 | 84.261 | -5.579  | 1.00 | 14.05 |
| ATOM | 789 | CB  | PHE A | 103 | 10.561 | 84.710 | -6.928  | 1.00 | 11.82 |
| ATOM | 790 | CG  | PHE A | 103 | 9.644  | 85.913 | -6.849  | 1.00 | 14.83 |
| ATOM | 791 | CD1 | PHE A | 103 | 10.149 | 87.189 | -6.601  | 1.00 | 16.95 |
| ATOM | 792 | CD2 | PHE A | 103 | 8.279  | 85.773 | -7.081  | 1.00 | 11.21 |
| ATOM | 793 | CE1 | PHE A | 103 | 9.295  | 88.309 | -6.583  | 1.00 | 12.90 |
| ATOM | 794 | CE2 | PHE A | 103 | 7.425  | 86.879 | -7.065  | 1.00 | 10.94 |
| ATOM | 795 | CZ  | PHE A | 103 | 7.936  | 88.146 | -6.820  | 1.00 | 12.78 |
| ATOM | 796 | C   | PHE A | 103 | 10.004 | 83.930 | -4.607  | 1.00 | 14.85 |
| ATOM | 797 | O   | PHE A | 103 | 9.249  | 82.981 | -4.822  | 1.00 | 14.06 |
| ATOM | 798 | N   | CYS A | 104 | 9.887  | 84.710 | -3.543  | 1.00 | 14.45 |
| ATOM | 799 | CA  | CYS A | 104 | 8.853  | 84.484 | -2.548  | 1.00 | 14.61 |

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|      |     |                |       |     |        |         |        |      |       |
|------|-----|----------------|-------|-----|--------|---------|--------|------|-------|
| ATOM | 800 | C <sub>2</sub> | CYS A | 104 | 9.509  | 84.235  | -1.194 | 1.00 | 14.79 |
| ATOM | 801 | SG             | CYS A | 104 | 8.386  | 84.134  | 0.215  | 1.00 | 18.12 |
| ATOM | 802 | C              | CYS A | 104 | 7.896  | 85.662  | -2.429 | 1.00 | 18.09 |
| ATOM | 803 | O              | CYS A | 104 | 8.322  | 86.821  | -2.482 | 1.00 | 18.91 |
| ATOM | 804 | N              | TYR A | 105 | 6.600  | 85.367  | -2.339 | 1.00 | 17.06 |
| ATOM | 805 | CA             | TYR A | 105 | 5.594  | 86.403  | -2.161 | 1.00 | 13.87 |
| ATOM | 806 | CB             | TYR A | 105 | 4.941  | 86.845  | -3.486 | 1.00 | 12.35 |
| ATOM | 807 | CG             | TYR A | 105 | 4.103  | 85.830  | -4.234 | 1.00 | 14.43 |
| ATOM | 808 | CD1            | TYR A | 105 | 2.713  | 85.826  | -4.110 | 1.00 | 9.55  |
| ATOM | 809 | CE1            | TYR A | 105 | 1.927  | 84.933  | -4.832 | 1.00 | 7.61  |
| ATOM | 810 | CD2            | TYR A | 105 | 4.690  | 84.909  | -5.112 | 1.00 | 11.05 |
| ATOM | 811 | CE2            | TYR A | 105 | 3.906  | 84.010  | -5.846 | 1.00 | 13.52 |
| ATOM | 812 | CZ             | TYR A | 105 | 2.525  | 84.028  | -5.699 | 1.00 | 15.44 |
| ATOM | 813 | OH             | TYR A | 105 | 1.733  | 83.129  | -6.395 | 1.00 | 18.33 |
| ATOM | 814 | C              | TYR A | 105 | 4.576  | 85.967  | -1.100 | 1.00 | 17.62 |
| ATOM | 815 | O              | TYR A | 105 | 4.412  | 84.773  | -0.820 | 1.00 | 14.49 |
| ATOM | 816 | N              | LEU A | 106 | 3.991  | 86.954  | -0.432 | 1.00 | 18.67 |
| ATOM | 817 | CA             | LEU A | 106 | 3.031  | 86.742  | 0.640  | 1.00 | 17.72 |
| ATOM | 818 | CB             | LEU A | 106 | 3.437  | 87.602  | 1.844  | 1.00 | 15.11 |
| ATOM | 819 | CG             | LEU A | 106 | 4.930  | 87.554  | 2.171  | 1.00 | 18.61 |
| ATOM | 820 | CD1            | LEU A | 106 | 5.237  | 88.376  | 3.384  | 1.00 | 20.22 |
| ATOM | 821 | CD2            | LEU A | 106 | 5.358  | 86.124  | 2.391  | 1.00 | 19.75 |
| ATOM | 822 | C              | LEU A | 106 | 1.594  | 87.078  | 0.237  | 1.00 | 19.55 |
| ATOM | 823 | O              | LEU A | 106 | 1.266  | 87.191  | -0.947 | 1.00 | 19.69 |
| ATOM | 824 | N              | ASN A | 107 | 0.753  | 87.241  | 1.253  | 1.00 | 16.25 |
| ATOM | 825 | CA             | ASN A | 107 | -0.659 | 87.563  | 1.122  | 1.00 | 18.19 |
| ATOM | 826 | CB             | ASN A | 107 | -1.231 | 87.792  | 2.518  | 1.00 | 24.35 |
| ATOM | 827 | CG             | ASN A | 107 | -2.738 | 87.979  | 2.530  | 1.00 | 22.21 |
| ATOM | 828 | OD1            | ASN A | 107 | -3.332 | 88.525  | 1.591  | 1.00 | 16.86 |
| ATOM | 829 | ND2            | ASN A | 107 | -3.362 | 87.551  | 3.618  | 1.00 | 15.33 |
| ATOM | 830 | C              | ASN A | 107 | -0.817 | 88.812  | 0.279  | 1.00 | 16.38 |
| ATOM | 831 | O              | ASN A | 107 | -0.332 | 89.888  | 0.634  | 1.00 | 14.14 |
| ATOM | 832 | N              | PRO A | 108 | -1.497 | 88.686  | -0.860 | 1.00 | 13.05 |
| ATOM | 833 | CD             | PRO A | 108 | -1.973 | 87.430  | -1.466 | 1.00 | 14.52 |
| ATOM | 834 | CA             | PRO A | 108 | -1.712 | 89.818  | -1.757 | 1.00 | 11.78 |
| ATOM | 835 | CB             | PRO A | 108 | -2.552 | 89.206  | -2.867 | 1.00 | 13.10 |
| ATOM | 836 | CG             | PRO A | 108 | -2.018 | 87.779  | -2.916 | 1.00 | 15.10 |
| ATOM | 837 | C              | PRO A | 108 | -2.409 | 91.006  | -1.113 | 1.00 | 15.99 |
| ATOM | 838 | O              | PRO A | 108 | -2.295 | 92.126  | -1.595 | 1.00 | 16.27 |
| ATOM | 839 | N              | ASN A | 109 | -3.114 | 90.776  | -0.014 | 1.00 | 18.12 |
| ATOM | 840 | CA             | ASN A | 109 | -3.838 | 91.855  | 0.649  | 1.00 | 17.89 |
| ATOM | 841 | CB             | ASN A | 109 | -5.005 | 91.304  | 1.461  | 1.00 | 15.82 |
| ATOM | 842 | CG             | ASN A | 109 | -6.058 | 90.695  | 0.590  | 1.00 | 18.28 |
| ATOM | 843 | OD1            | ASN A | 109 | -6.374 | 91.228  | -0.475 | 1.00 | 14.24 |
| ATOM | 844 | ND2            | ASN A | 109 | -6.578 | 89.549  | 1.001  | 1.00 | 19.06 |
| ATOM | 845 | C              | ASN A | 109 | -2.990 | 92.759  | 1.511  | 1.00 | 22.19 |
| ATOM | 846 | O              | ASN A | 109 | -3.467 | 93.786  | 1.978  | 1.00 | 17.26 |
| ATOM | 847 | N              | PHE A | 110 | -1.762 | 92.349  | 1.791  | 1.00 | 13.51 |
| ATOM | 848 | CA             | PHE A | 110 | -0.879 | 93.168  | 2.588  | 1.00 | 11.28 |
| ATOM | 849 | CB             | PHE A | 110 | 0.304  | 92.345  | 3.068  | 1.00 | 14.89 |
| ATOM | 850 | CG             | PHE A | 110 | -0.054 | 91.343  | 4.110  | 1.00 | 14.80 |
| ATOM | 851 | CD1            | PHE A | 110 | -1.296 | 91.384  | 4.727  | 1.00 | 16.71 |
| ATOM | 852 | CD2            | PHE A | 110 | 0.854  | 90.365  | 4.494  | 1.00 | 15.38 |
| ATOM | 853 | CE1            | PHE A | 110 | -1.627 | 90.470  | 5.702  | 1.00 | 14.69 |
| ATOM | 854 | CE2            | PHE A | 110 | 0.532  | 89.440  | 5.474  | 1.00 | 18.74 |
| ATOM | 855 | CZ             | PHE A | 110 | -0.710 | 89.495  | 6.082  | 1.00 | 16.88 |
| ATOM | 856 | C              | PHE A | 110 | -0.404 | 94.363  | 1.787  | 1.00 | 21.88 |
| ATOM | 857 | O              | PHE A | 110 | 0.469  | 94.243  | 0.930  | 1.00 | 18.68 |
| ATOM | 858 | N              | THR A | 111 | -1.032 | 95.509  | 2.004  | 1.00 | 16.37 |
| ATOM | 859 | CA             | THR A | 111 | -0.625 | 96.718  | 1.304  | 1.00 | 15.54 |
| ATOM | 860 | CB             | THR A | 111 | -1.764 | 97.305  | 0.482  | 1.00 | 18.30 |
| ATOM | 861 | OG1            | THR A | 111 | -2.723 | 97.911  | 1.355  | 1.00 | 11.84 |
| ATOM | 862 | CG2            | THR A | 111 | -2.423 | 96.221  | -0.337 | 1.00 | 18.43 |
| ATOM | 863 | C              | THR A | 111 | -0.219 | 97.692  | 2.389  | 1.00 | 23.70 |
| ATOM | 864 | O              | THR A | 111 | -0.284 | 97.360  | 3.564  | 1.00 | 21.65 |
| ATOM | 865 | N              | PRO A | 112 | 0.229  | 98.895  | 2.023  | 1.00 | 15.84 |
| ATOM | 866 | CD             | PRO A | 112 | 0.707  | 99.351  | 0.703  | 1.00 | 23.93 |
| ATOM | 867 | CA             | PRO A | 112 | 0.626  | 99.845  | 3.069  | 1.00 | 21.58 |
| ATOM | 868 | CB             | PRO A | 112 | 1.273  | 100.969 | 2.272  | 1.00 | 19.10 |
| ATOM | 869 | CG             | PRO A | 112 | 1.847  | 100.236 | 1.079  | 1.00 | 28.77 |
| ATOM | 870 | C              | PRO A | 112 | -0.507 | 100.371 | 3.954  | 1.00 | 34.33 |
| ATOM | 871 | O              | PRO A | 112 | -0.245 | 100.991 | 4.981  | 1.00 | 30.89 |
| ATOM | 872 | N              | ASP A | 113 | -1.756 | 100.137 | 3.557  | 1.00 |       |

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|      |     |     |       |     |        |         |        |      |       |
|------|-----|-----|-------|-----|--------|---------|--------|------|-------|
| ATOM | 873 | CA  | ASP A | 113 | -2.908 | 100.608 | 4.325  | 1.00 | 29.23 |
| ATOM | 874 | CB  | ASP A | 113 | -4.095 | 100.876 | 3.403  | 1.00 | 33.62 |
| ATOM | 875 | CG  | ASP A | 113 | -3.740 | 101.759 | 2.229  | 1.00 | 39.32 |
| ATOM | 876 | OD1 | ASP A | 113 | -3.551 | 102.980 | 2.420  | 1.00 | 38.82 |
| ATOM | 877 | OD2 | ASP A | 113 | -3.659 | 101.220 | 1.107  | 1.00 | 41.64 |
| ATOM | 878 | C   | ASP A | 113 | -3.313 | 99.552  | 5.330  | 1.00 | 26.58 |
| ATOM | 879 | O   | ASP A | 113 | -4.020 | 99.831  | 6.288  | 1.00 | 30.47 |
| ATOM | 880 | N   | HIS A | 114 | -2.875 | 98.327  | 5.090  | 1.00 | 22.11 |
| ATOM | 881 | CA  | HIS A | 114 | -3.203 | 97.223  | 5.964  | 1.00 | 18.51 |
| ATOM | 882 | CB  | HIS A | 114 | -2.562 | 95.954  | 5.434  | 1.00 | 18.88 |
| ATOM | 883 | CG  | HIS A | 114 | -3.154 | 94.695  | 5.980  | 1.00 | 20.47 |
| ATOM | 884 | CD2 | HIS A | 114 | -3.955 | 93.771  | 5.401  | 1.00 | 20.61 |
| ATOM | 885 | ND1 | HIS A | 114 | -2.905 | 94.243  | 7.255  | 1.00 | 21.89 |
| ATOM | 886 | CE1 | HIS A | 114 | -3.527 | 93.092  | 7.440  | 1.00 | 20.69 |
| ATOM | 887 | NE2 | HIS A | 114 | -4.170 | 92.784  | 6.331  | 1.00 | 16.26 |
| ATOM | 888 | C   | HIS A | 114 | -2.682 | 97.529  | 7.347  | 1.00 | 20.91 |
| ATOM | 889 | O   | HIS A | 114 | -1.511 | 97.821  | 7.518  | 1.00 | 23.53 |
| ATOM | 890 | N   | PRO A | 115 | -3.535 | 97.414  | 8.365  | 1.00 | 23.07 |
| ATOM | 891 | CD  | PRO A | 115 | -4.933 | 96.973  | 8.311  | 1.00 | 24.88 |
| ATOM | 892 | CA  | PRO A | 115 | -3.148 | 97.688  | 9.745  | 1.00 | 24.93 |
| ATOM | 893 | CB  | PRO A | 115 | -4.411 | 97.334  | 10.525 | 1.00 | 27.48 |
| ATOM | 894 | CG  | PRO A | 115 | -5.094 | 96.342  | 9.652  | 1.00 | 24.00 |
| ATOM | 895 | C   | PRO A | 115 | -1.927 | 96.923  | 10.233 | 1.00 | 26.06 |
| ATOM | 896 | O   | PRO A | 115 | -1.127 | 97.456  | 10.991 | 1.00 | 32.32 |
| ATOM | 897 | N   | ARG A | 116 | -1.782 | 95.678  | 9.802  | 1.00 | 26.43 |
| ATOM | 898 | CA  | ARG A | 116 | -0.634 | 94.868  | 10.199 | 1.00 | 26.26 |
| ATOM | 899 | CB  | ARG A | 116 | -0.810 | 93.430  | 9.727  | 1.00 | 30.69 |
| ATOM | 900 | CG  | ARG A | 116 | -1.813 | 92.629  | 10.516 | 1.00 | 35.60 |
| ATOM | 901 | CD  | ARG A | 116 | -1.372 | 92.533  | 11.950 | 1.00 | 39.57 |
| ATOM | 902 | NE  | ARG A | 116 | -2.151 | 91.547  | 12.685 | 1.00 | 44.77 |
| ATOM | 903 | CZ  | ARG A | 116 | -2.021 | 91.314  | 13.988 | 1.00 | 47.07 |
| ATOM | 904 | NH1 | ARG A | 116 | -1.145 | 91.997  | 14.721 | 1.00 | 44.22 |
| ATOM | 905 | NH2 | ARG A | 116 | -2.758 | 90.379  | 14.556 | 1.00 | 46.39 |
| ATOM | 906 | C   | ARG A | 116 | 0.681  | 95.416  | 9.653  | 1.00 | 27.56 |
| ATOM | 907 | O   | ARG A | 116 | 1.727  | 95.273  | 10.276 | 1.00 | 28.41 |
| ATOM | 908 | N   | ILE A | 117 | 0.624  | 96.021  | 8.473  | 1.00 | 28.17 |
| ATOM | 909 | CA  | ILE A | 117 | 1.806  | 96.580  | 7.835  | 1.00 | 28.31 |
| ATOM | 910 | CB  | ILE A | 117 | 1.584  | 96.734  | 6.307  | 1.00 | 24.00 |
| ATOM | 911 | CG2 | ILE A | 117 | 2.790  | 97.357  | 5.644  | 1.00 | 23.25 |
| ATOM | 912 | CG1 | ILE A | 117 | 1.315  | 95.372  | 5.668  | 1.00 | 20.98 |
| ATOM | 913 | CD1 | ILE A | 117 | 2.506  | 94.482  | 5.596  | 1.00 | 16.97 |
| ATOM | 914 | C   | ILE A | 117 | 2.140  | 97.930  | 8.490  | 1.00 | 34.06 |
| ATOM | 915 | O   | ILE A | 117 | 3.308  | 98.237  | 8.742  | 1.00 | 40.01 |
| ATOM | 916 | N   | GLN A | 118 | 1.111  | 98.716  | 8.797  | 1.00 | 34.32 |
| ATOM | 917 | CA  | GLN A | 118 | 1.289  | 100.008 | 9.446  | 1.00 | 31.25 |
| ATOM | 918 | CB  | GLN A | 118 | -0.036 | 100.751 | 9.510  | 1.00 | 32.56 |
| ATOM | 919 | CG  | GLN A | 118 | -0.532 | 101.215 | 8.175  | 1.00 | 41.97 |
| ATOM | 920 | CD  | GLN A | 118 | -1.790 | 102.040 | 8.289  | 1.00 | 49.04 |
| ATOM | 921 | OE1 | GLN A | 118 | -2.349 | 102.203 | 9.374  | 1.00 | 54.55 |
| ATOM | 922 | NE2 | GLN A | 118 | -2.241 | 102.577 | 7.167  | 1.00 | 54.77 |
| ATOM | 923 | C   | GLN A | 118 | 1.813  | 99.816  | 10.857 | 1.00 | 30.00 |
| ATOM | 924 | O   | GLN A | 118 | 2.606  | 100.602 | 11.348 | 1.00 | 36.36 |
| ATOM | 925 | N   | ALA A | 119 | 1.362  | 98.759  | 11.506 | 1.00 | 27.04 |
| ATOM | 926 | CA  | ALA A | 119 | 1.801  | 98.470  | 12.851 | 1.00 | 23.94 |
| ATOM | 927 | CB  | ALA A | 119 | 0.898  | 97.447  | 13.457 | 1.00 | 23.97 |
| ATOM | 928 | C   | ALA A | 119 | 3.223  | 97.944  | 12.836 | 1.00 | 29.31 |
| ATOM | 929 | O   | ALA A | 119 | 3.839  | 97.802  | 13.885 | 1.00 | 35.94 |
| ATOM | 930 | N   | LYS A | 120 | 3.728  | 97.625  | 11.649 | 1.00 | 30.68 |
| ATOM | 931 | CA  | LYS A | 120 | 5.068  | 97.075  | 11.497 | 1.00 | 31.26 |
| ATOM | 932 | CB  | LYS A | 120 | 6.131  | 98.127  | 11.815 | 1.00 | 32.35 |
| ATOM | 933 | CG  | LYS A | 120 | 6.210  | 99.208  | 10.756 | 1.00 | 41.07 |
| ATOM | 934 | CD  | LYS A | 120 | 7.461  | 100.047 | 10.893 | 1.00 | 53.39 |
| ATOM | 935 | CE  | LYS A | 120 | 7.720  | 100.864 | 9.621  | 1.00 | 60.71 |
| ATOM | 936 | NZ  | LYS A | 120 | 9.046  | 101.563 | 9.644  | 1.00 | 65.99 |
| ATOM | 937 | C   | LYS A | 120 | 5.271  | 95.796  | 12.321 | 1.00 | 30.21 |
| ATOM | 938 | O   | LYS A | 120 | 6.266  | 95.633  | 13.014 | 1.00 | 34.12 |
| ATOM | 939 | N   | THR A | 121 | 4.287  | 94.901  | 12.240 | 1.00 | 30.59 |
| ATOM | 940 | CA  | THR A | 121 | 4.304  | 93.627  | 12.945 | 1.00 | 29.59 |
| ATOM | 941 | CB  | THR A | 121 | 2.897  | 93.001  | 12.953 | 1.00 | 26.01 |
| ATOM | 942 | OG1 | THR A | 121 | 1.948  | 93.993  | 13.347 | 1.00 | 29.93 |
| ATOM | 943 | CG2 | THR A | 121 | 2.830  | 91.841  | 13.924 | 1.00 | 27.80 |
| ATOM | 944 | C   | THR A | 21  | 5.238  | 92.685  | 12.203 | 1.00 | 31.22 |
| ATOM | 945 | O   | THR A | 121 | 5.258  | 92.684  | 10.977 | 1.00 | 36.88 |

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|      |      |     |       |     |       |        |         |      |       |
|------|------|-----|-------|-----|-------|--------|---------|------|-------|
| ATOM | 946  | N   | PRO A | 122 | 6.016 | 91.867 | 12.918  | 1.00 | 31.48 |
| ATOM | 947  | CD  | PRO A | 122 | 6.173 | 91.788 | 14.375  | 1.00 | 30.51 |
| ATOM | 948  | CA  | PRO A | 122 | 6.936 | 90.939 | 12.260  | 1.00 | 29.39 |
| ATOM | 949  | CB  | PRO A | 122 | 7.519 | 90.162 | 13.428  | 1.00 | 28.00 |
| ATOM | 950  | CG  | PRO A | 122 | 7.524 | 91.147 | 14.508  | 1.00 | 28.89 |
| ATOM | 951  | C   | PRO A | 122 | 6.213 | 89.993 | 11.324  | 1.00 | 29.95 |
| ATOM | 952  | O   | PRO A | 122 | 5.017 | 89.759 | 11.499  | 1.00 | 33.22 |
| ATOM | 953  | N   | THR A | 123 | 6.957 | 89.422 | 10.373  | 1.00 | 30.79 |
| ATOM | 954  | CA  | THR A | 123 | 6.470 | 88.472 | 9.355   | 1.00 | 28.32 |
| ATOM | 955  | CB  | THR A | 123 | 5.859 | 87.189 | 9.961   | 1.00 | 30.03 |
| ATOM | 956  | OG1 | THR A | 123 | 4.648 | 87.498 | 10.661  | 1.00 | 35.13 |
| ATOM | 957  | CG2 | THR A | 123 | 6.835 | 86.507 | 10.897  | 1.00 | 31.48 |
| ATOM | 958  | C   | THR A | 123 | 5.505 | 89.028 | 8.309   | 1.00 | 27.79 |
| ATOM | 959  | O   | THR A | 123 | 5.164 | 88.310 | 7.377   | 1.00 | 29.06 |
| ATOM | 960  | N   | HIS A | 124 | 5.076 | 90.285 | 8.458   | 1.00 | 24.80 |
| ATOM | 961  | CA  | HIS A | 124 | 4.150 | 90.920 | 7.504   | 1.00 | 22.12 |
| ATOM | 962  | CB  | HIS A | 124 | 3.072 | 91.740 | 8.226   | 1.00 | 17.07 |
| ATOM | 963  | CG  | HIS A | 124 | 2.285 | 90.948 | 9.215   | 1.00 | 13.05 |
| ATOM | 964  | CD2 | HIS A | 124 | 1.035 | 90.435 | 9.145   | 1.00 | 18.78 |
| ATOM | 965  | ND1 | HIS A | 124 | 2.798 | 90.529 | 10.420  | 1.00 | 15.62 |
| ATOM | 966  | CE1 | HIS A | 124 | 1.907 | 89.785 | 11.044  | 1.00 | 17.88 |
| ATOM | 967  | NE2 | HIS A | 124 | 0.825 | 89.712 | 10.292  | 1.00 | 17.44 |
| ATOM | 968  | C   | HIS A | 124 | 4.941 | 91.837 | 6.592   | 1.00 | 21.71 |
| ATOM | 969  | O   | HIS A | 124 | 5.645 | 92.715 | 7.050   | 1.00 | 22.54 |
| ATOM | 970  | N   | GLU A | 125 | 4.819 | 91.632 | 5.295   | 1.00 | 21.78 |
| ATOM | 971  | CA  | GLU A | 125 | 5.538 | 92.456 | 4.339   | 1.00 | 20.92 |
| ATOM | 972  | CB  | GLU A | 125 | 6.787 | 91.730 | 3.852   | 1.00 | 23.07 |
| ATOM | 973  | CG  | GLU A | 125 | 8.023 | 91.998 | 4.651   | 1.00 | 24.04 |
| ATOM | 974  | CD  | GLU A | 125 | 9.169 | 91.132 | 4.222   | 1.00 | 24.79 |
| ATOM | 975  | OE1 | GLU A | 125 | 9.457 | 91.049 | 3.012   | 1.00 | 24.03 |
| ATOM | 976  | OE2 | GLU A | 125 | 9.793 | 90.539 | 5.107   | 1.00 | 31.23 |
| ATOM | 977  | C   | GLU A | 125 | 4.668 | 92.738 | 3.143   | 1.00 | 21.05 |
| ATOM | 978  | O   | GLU A | 125 | 3.660 | 92.080 | 2.930   | 1.00 | 24.62 |
| ATOM | 979  | N   | VAL A | 126 | 5.091 | 93.694 | 2.339   | 1.00 | 21.65 |
| ATOM | 980  | CA  | VAL A | 126 | 4.361 | 94.031 | 1.146   | 1.00 | 22.78 |
| ATOM | 981  | CB  | VAL A | 126 | 4.203 | 95.538 | 1.042   | 1.00 | 20.08 |
| ATOM | 982  | CG1 | VAL A | 126 | 3.508 | 95.900 | -0.229  | 1.00 | 17.38 |
| ATOM | 983  | CG2 | VAL A | 126 | 3.405 | 96.028 | 2.228   | 1.00 | 20.49 |
| ATOM | 984  | C   | VAL A | 126 | 5.166 | 93.459 | -0.019  | 1.00 | 25.89 |
| ATOM | 985  | O   | VAL A | 126 | 6.380 | 93.667 | -0.099  | 1.00 | 30.48 |
| ATOM | 986  | N   | ASN A | 127 | 4.511 | 92.683 | -0.880  | 1.00 | 21.77 |
| ATOM | 987  | CA  | ASN A | 127 | 5.174 | 92.053 | -2.020  | 1.00 | 19.25 |
| ATOM | 988  | CB  | ASN A | 127 | 4.182 | 91.207 | -2.830  | 1.00 | 18.25 |
| ATOM | 989  | CG  | ASN A | 127 | 3.724 | 89.985 | -2.095  | 1.00 | 16.94 |
| ATOM | 990  | OD1 | ASN A | 127 | 4.459 | 89.445 | -1.286  | 1.00 | 16.08 |
| ATOM | 991  | ND2 | ASN A | 127 | 2.512 | 89.528 | -2.380  | 1.00 | 12.62 |
| ATOM | 992  | C   | ASN A | 127 | 5.857 | 93.007 | -2.975  | 1.00 | 19.23 |
| ATOM | 993  | O   | ASN A | 127 | 5.436 | 94.150 | -3.148  | 1.00 | 19.59 |
| ATOM | 994  | N   | VAL A | 128 | 6.948 | 92.525 | -3.556  | 1.00 | 18.95 |
| ATOM | 995  | CA  | VAL A | 128 | 7.698 | 93.260 | -4.561  | 1.00 | 23.17 |
| ATOM | 996  | CB  | VAL A | 128 | 9.228 | 93.403 | -4.235  | 1.00 | 21.82 |
| ATOM | 997  | CG1 | VAL A | 128 | 9.427 | 94.284 | -3.027  | 1.00 | 20.58 |
| ATOM | 998  | CG2 | VAL A | 128 | 9.880 | 92.055 | -3.999  | 1.00 | 23.71 |
| ATOM | 999  | C   | VAL A | 128 | 7.494 | 92.408 | -5.808  | 1.00 | 23.82 |
| ATOM | 1000 | O   | VAL A | 128 | 7.486 | 91.183 | -5.730  | 1.00 | 23.35 |
| ATOM | 1001 | N   | TRP A | 129 | 7.312 | 93.050 | -6.951  | 1.00 | 25.96 |
| ATOM | 1002 | CA  | TRP A | 129 | 7.066 | 92.319 | -8.179  | 1.00 | 28.04 |
| ATOM | 1003 | CB  | TRP A | 129 | 5.604 | 92.476 | -8.562  | 1.00 | 22.71 |
| ATOM | 1004 | CG  | TRP A | 129 | 4.646 | 91.925 | -7.588  | 1.00 | 20.42 |
| ATOM | 1005 | CD2 | TRP A | 129 | 4.254 | 90.557 | -7.467  | 1.00 | 17.81 |
| ATOM | 1006 | CE2 | TRP A | 129 | 3.222 | 90.505 | -6.508  | 1.00 | 16.80 |
| ATOM | 1007 | CE3 | TRP A | 129 | 4.667 | 89.371 | -8.084  | 1.00 | 17.14 |
| ATOM | 1008 | CD1 | TRP A | 129 | 3.873 | 92.629 | -6.710  | 1.00 | 15.97 |
| ATOM | 1009 | NE1 | TRP A | 129 | 3.008 | 91.784 | -6.063  | 1.00 | 17.97 |
| ATOM | 1010 | CZ2 | TRP A | 129 | 2.597 | 89.313 | -6.155  | 1.00 | 19.47 |
| ATOM | 1011 | CZ3 | TRP A | 129 | 4.048 | 88.188 | -7.734  | 1.00 | 16.93 |
| ATOM | 1012 | CH2 | TRP A | 129 | 3.024 | 88.167 | -6.780  | 1.00 | 18.76 |
| ATOM | 1013 | C   | TRP A | 129 | 7.887 | 92.838 | -9.336  | 1.00 | 30.23 |
| ATOM | 1014 | O   | TRP A | 129 | 8.323 | 93.985 | -9.325  | 1.00 | 30.92 |
| ATOM | 1015 | N   | PRO A | 130 | 8.103 | 92.000 | -10.361 | 1.00 | 32.08 |
| ATOM | 1016 | CD  | PRO A | 130 | 7.807 | 90.562 | -10.498 | 1.00 | 31.53 |
| ATOM | 1017 | CA  | PRO A | 130 | 8.880 | 92.474 | -11.503 | 1.00 | 33.41 |
| ATOM | 1018 | CB  | PRO A | 130 | 9.109 | 91.192 | -12.308 | 1.00 | 31.40 |

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|      |      |     |       |     |        |        |         |      |       |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 1019 | CG  | PRO A | 130 | 7.926  | 90.364 | -11.986 | 1.00 | 28.64 |
| ATOM | 1020 | C   | PRO A | 130 | 8.090  | 93.521 | -12.298 | 1.00 | 35.25 |
| ATOM | 1021 | O   | PRO A | 130 | 6.869  | 93.651 | -12.146 | 1.00 | 36.95 |
| ATOM | 1022 | N   | ASP A | 131 | 8.805  | 94.301 | -13.100 | 1.00 | 38.98 |
| ATOM | 1023 | CA  | ASP A | 131 | 8.185  | 95.329 | -13.927 | 1.00 | 41.94 |
| ATOM | 1024 | CB  | ASP A | 131 | 9.270  | 96.081 | -14.699 | 1.00 | 49.89 |
| ATOM | 1025 | CG  | ASP A | 131 | 8.713  | 97.168 | -15.612 | 1.00 | 59.35 |
| ATOM | 1026 | OD1 | ASP A | 131 | 7.519  | 97.540 | -15.503 | 1.00 | 60.33 |
| ATOM | 1027 | OD2 | ASP A | 131 | 9.499  | 97.667 | -16.448 | 1.00 | 69.02 |
| ATOM | 1028 | C   | ASP A | 131 | 7.160  | 94.732 | -14.895 | 1.00 | 40.13 |
| ATOM | 1029 | O   | ASP A | 131 | 7.444  | 93.761 | -15.604 | 1.00 | 39.39 |
| ATOM | 1030 | N   | GLU A | 132 | 5.983  | 95.343 | -14.933 | 1.00 | 38.57 |
| ATOM | 1031 | CA  | GLU A | 132 | 4.895  | 94.906 | -15.796 | 1.00 | 41.66 |
| ATOM | 1032 | CB  | GLU A | 132 | 3.675  | 95.805 | -15.594 | 1.00 | 49.43 |
| ATOM | 1033 | CG  | GLU A | 132 | 2.565  | 95.210 | -14.742 | 1.00 | 63.43 |
| ATOM | 1034 | CD  | GLU A | 132 | 1.767  | 94.123 | -15.455 | 1.00 | 68.77 |
| ATOM | 1035 | OE1 | GLU A | 132 | 1.390  | 93.130 | -14.786 | 1.00 | 73.49 |
| ATOM | 1036 | OE2 | GLU A | 132 | 1.501  | 94.268 | -16.671 | 1.00 | 70.44 |
| ATOM | 1037 | C   | GLU A | 132 | 5.249  | 94.919 | -17.269 | 1.00 | 40.84 |
| ATOM | 1038 | O   | GLU A | 132 | 4.925  | 93.984 | -17.998 | 1.00 | 42.27 |
| ATOM | 1039 | N   | THR A | 133 | 5.909  | 95.984 | -17.709 | 1.00 | 40.91 |
| ATOM | 1040 | CA  | THR A | 133 | 6.261  | 96.124 | -19.114 | 1.00 | 42.12 |
| ATOM | 1041 | CB  | THR A | 133 | 7.100  | 97.407 | -19.373 | 1.00 | 43.93 |
| ATOM | 1042 | OG1 | THR A | 133 | 8.431  | 97.217 | -18.884 | 1.00 | 56.48 |
| ATOM | 1043 | CG2 | THR A | 133 | 6.496  | 98.602 | -18.650 | 1.00 | 42.47 |
| ATOM | 1044 | C   | THR A | 133 | 7.045  | 94.908 | -19.576 | 1.00 | 40.83 |
| ATOM | 1045 | O   | THR A | 133 | 6.800  | 94.369 | -20.650 | 1.00 | 45.82 |
| ATOM | 1046 | N   | LYS A | 134 | 7.945  | 94.450 | -18.717 | 1.00 | 40.62 |
| ATOM | 1047 | CA  | LYS A | 134 | 8.799  | 93.312 | -19.014 | 1.00 | 40.68 |
| ATOM | 1048 | CB  | LYS A | 134 | 10.109 | 93.429 | -18.233 | 1.00 | 44.31 |
| ATOM | 1049 | CG  | LYS A | 134 | 10.852 | 94.742 | -18.437 | 1.00 | 50.92 |
| ATOM | 1050 | CD  | LYS A | 134 | 12.171 | 94.754 | -17.681 | 1.00 | 56.36 |
| ATOM | 1051 | CE  | LYS A | 134 | 12.883 | 96.096 | -17.809 | 1.00 | 64.21 |
| ATOM | 1052 | NZ  | LYS A | 134 | 14.159 | 96.104 | -17.026 | 1.00 | 72.09 |
| ATOM | 1053 | C   | LYS A | 134 | 8.176  | 91.950 | -18.737 | 1.00 | 40.31 |
| ATOM | 1054 | O   | LYS A | 134 | 8.563  | 90.955 | -19.348 | 1.00 | 45.00 |
| ATOM | 1055 | N   | HIS A | 135 | 7.278  | 91.875 | -17.763 | 1.00 | 38.10 |
| ATOM | 1056 | CA  | HIS A | 135 | 6.649  | 90.601 | -17.425 | 1.00 | 34.82 |
| ATOM | 1057 | CB  | HIS A | 135 | 7.200  | 90.071 | -16.089 | 1.00 | 28.65 |
| ATOM | 1058 | CG  | HIS A | 135 | 8.654  | 89.705 | -16.124 | 1.00 | 21.40 |
| ATOM | 1059 | CD2 | HIS A | 135 | 9.267  | 88.523 | -16.373 | 1.00 | 22.41 |
| ATOM | 1060 | ND1 | HIS A | 135 | 9.659  | 90.614 | -15.880 | 1.00 | 21.96 |
| ATOM | 1061 | CE1 | HIS A | 135 | 10.832 | 90.012 | -15.978 | 1.00 | 21.23 |
| ATOM | 1062 | NE2 | HIS A | 135 | 10.624 | 88.743 | -16.276 | 1.00 | 26.04 |
| ATOM | 1063 | C   | HIS A | 135 | 5.135  | 90.787 | -17.335 | 1.00 | 37.00 |
| ATOM | 1064 | O   | HIS A | 135 | 4.536  | 90.584 | -16.271 | 1.00 | 36.99 |
| ATOM | 1065 | N   | PRO A | 136 | 4.489  | 91.128 | -18.465 | 1.00 | 38.00 |
| ATOM | 1066 | CD  | PRO A | 136 | 5.065  | 91.093 | -19.820 | 1.00 | 39.72 |
| ATOM | 1067 | CA  | PRO A | 136 | 3.043  | 91.352 | -18.545 | 1.00 | 35.57 |
| ATOM | 1068 | CB  | PRO A | 136 | 2.801  | 91.478 | -20.048 | 1.00 | 33.63 |
| ATOM | 1069 | CG  | PRO A | 136 | 3.882  | 90.651 | -20.639 | 1.00 | 35.65 |
| ATOM | 1070 | C   | PRO A | 136 | 2.183  | 90.264 | -17.935 | 1.00 | 33.54 |
| ATOM | 1071 | O   | PRO A | 136 | 2.348  | 89.083 | -18.231 | 1.00 | 35.53 |
| ATOM | 1072 | N   | GLY A | 137 | 1.284  | 90.680 | -17.053 | 1.00 | 33.66 |
| ATOM | 1073 | CA  | GLY A | 137 | 0.379  | 89.753 | -16.408 | 1.00 | 35.45 |
| ATOM | 1074 | C   | GLY A | 137 | 0.946  | 88.810 | -15.361 | 1.00 | 36.34 |
| ATOM | 1075 | O   | GLY A | 137 | 0.212  | 87.981 | -14.829 | 1.00 | 41.58 |
| ATOM | 1076 | N   | PHE A | 138 | 2.224  | 88.926 | -15.029 | 1.00 | 34.29 |
| ATOM | 1077 | CA  | PHE A | 138 | 2.792  | 88.034 | -14.022 | 1.00 | 32.30 |
| ATOM | 1078 | CB  | PHE A | 138 | 4.315  | 88.175 | -13.960 | 1.00 | 33.36 |
| ATOM | 1079 | CG  | PHE A | 138 | 4.960  | 87.272 | -12.959 | 1.00 | 29.73 |
| ATOM | 1080 | CD1 | PHE A | 138 | 4.770  | 85.902 | -13.026 | 1.00 | 31.50 |
| ATOM | 1081 | CD2 | PHE A | 138 | 5.718  | 87.796 | -11.924 | 1.00 | 30.02 |
| ATOM | 1082 | CE1 | PHE A | 138 | 5.322  | 85.061 | -12.070 | 1.00 | 32.69 |
| ATOM | 1083 | CE2 | PHE A | 138 | 6.272  | B6.974 | -10.965 | 1.00 | 30.29 |
| ATOM | 1084 | CZ  | PHE A | 138 | 6.075  | 85.600 | -11.035 | 1.00 | 33.63 |
| ATOM | 1085 | C   | PHE A | 138 | 2.178  | 88.259 | -12.639 | 1.00 | 31.05 |
| ATOM | 1086 | O   | PHE A | 138 | 1.653  | 87.323 | -12.029 | 1.00 | 29.39 |
| ATOM | 1087 | N   | GLN A | 139 | 2.205  | 89.502 | -12.169 | 1.00 | 26.99 |
| ATOM | 1088 | CA  | GLN A | 139 | 1.662  | 89.816 | -10.861 | 1.00 | 28.51 |
| ATOM | 1089 | CB  | GLN A | 139 | 1.751  | 91.314 | -10.581 | 1.00 | 23.97 |
| ATOM | 1090 | CG  | GLN A | 139 | 1.090  | 91.725 | -9.275  | 1.00 | 27.92 |
| ATOM | 1091 | CD  | GLN A | 139 | 1.192  | 93.216 | -8.982  | 1.00 | 32.88 |

|      |      |     |       |     |        |        |         |      |       |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 1092 | OE1 | GLN A | 139 | 1.943  | 93.950 | -9.632  | 1.00 | 32.97 |
| ATOM | 1093 | NE2 | GLN A | 139 | 0.440  | 93.668 | -7.987  | 1.00 | 31.33 |
| ATOM | 1094 | C   | GLN A | 139 | 0.222  | 89.332 | -10.734 | 1.00 | 33.84 |
| ATOM | 1095 | O   | GLN A | 139 | -0.126 | 88.663 | -9.754  | 1.00 | 36.68 |
| ATOM | 1096 | N   | ASP A | 140 | -0.592 | 89.609 | -11.752 | 1.00 | 37.09 |
| ATOM | 1097 | CA  | ASP A | 140 | -2.003 | 89.206 | -11.747 | 1.00 | 35.96 |
| ATOM | 1098 | CB  | ASP A | 140 | -2.736 | 89.776 | -12.972 | 1.00 | 40.62 |
| ATOM | 1099 | CG  | ASP A | 140 | -2.672 | 91.300 | -13.044 | 1.00 | 49.63 |
| ATOM | 1100 | OD1 | ASP A | 140 | -3.391 | 91.955 | -12.266 | 1.00 | 51.54 |
| ATOM | 1101 | OD2 | ASP A | 140 | -1.906 | 91.840 | -13.875 | 1.00 | 56.38 |
| ATOM | 1102 | C   | ASP A | 140 | -2.140 | 87.684 | -11.694 | 1.00 | 34.15 |
| ATOM | 1103 | O   | ASP A | 140 | -3.024 | 87.149 | -11.023 | 1.00 | 35.48 |
| ATOM | 1104 | N   | PHE A | 141 | -1.258 | 86.981 | -12.389 | 1.00 | 29.30 |
| ATOM | 1105 | CA  | PHE A | 141 | -1.305 | 85.530 | -12.373 | 1.00 | 29.22 |
| ATOM | 1106 | CB  | PHE A | 141 | -0.296 | 84.942 | -13.368 | 1.00 | 26.63 |
| ATOM | 1107 | CG  | PHE A | 141 | 0.113  | 83.526 | -13.051 | 1.00 | 32.93 |
| ATOM | 1108 | CD1 | PHE A | 141 | -0.721 | 82.456 | -13.364 | 1.00 | 37.47 |
| ATOM | 1109 | CD2 | PHE A | 141 | 1.312  | 83.263 | -12.388 | 1.00 | 36.97 |
| ATOM | 1110 | CE1 | PHE A | 141 | -0.373 | 81.143 | -13.016 | 1.00 | 37.55 |
| ATOM | 1111 | CE2 | PHE A | 141 | 1.667  | 81.956 | -12.035 | 1.00 | 37.91 |
| ATOM | 1112 | CZ  | PHE A | 141 | 0.821  | 80.895 | -12.349 | 1.00 | 36.70 |
| ATOM | 1113 | C   | PHE A | 141 | -0.971 | 85.033 | -10.969 | 1.00 | 31.10 |
| ATOM | 1114 | O   | PHE A | 141 | -1.720 | 84.264 | -10.369 | 1.00 | 34.39 |
| ATOM | 1115 | N   | ALA A | 142 | 0.162  | 85.493 | -10.454 | 1.00 | 27.56 |
| ATOM | 1116 | CA  | ALA A | 142 | 0.657  | 85.091 | -9.149  | 1.00 | 23.24 |
| ATOM | 1117 | CB  | ALA A | 142 | 1.969  | 85.792 | -8.880  | 1.00 | 26.02 |
| ATOM | 1118 | C   | ALA A | 142 | -0.317 | 85.313 | -7.995  | 1.00 | 23.50 |
| ATOM | 1119 | O   | ALA A | 142 | -0.438 | 84.480 | -7.094  | 1.00 | 23.30 |
| ATOM | 1120 | N   | GLU A | 143 | -1.013 | 86.437 | -8.022  | 1.00 | 24.11 |
| ATOM | 1121 | CA  | GLU A | 143 | -1.969 | 86.750 | -6.970  | 1.00 | 26.83 |
| ATOM | 1122 | CB  | GLU A | 143 | -2.403 | 88.211 | -7.077  | 1.00 | 27.46 |
| ATOM | 1123 | CG  | GLU A | 143 | -1.262 | 89.196 | -6.890  | 1.00 | 30.94 |
| ATOM | 1124 | CD  | GLU A | 143 | -1.733 | 90.618 | -6.681  | 1.00 | 36.67 |
| ATOM | 1125 | OE1 | GLU A | 143 | -0.906 | 91.448 | -6.250  | 1.00 | 40.24 |
| ATOM | 1126 | OE2 | GLU A | 143 | -2.921 | 90.916 | -6.943  | 1.00 | 40.10 |
| ATOM | 1127 | C   | GLU A | 143 | -3.183 | 85.824 | -7.018  | 1.00 | 29.25 |
| ATOM | 1128 | O   | GLU A | 143 | -3.640 | 85.318 | -5.989  | 1.00 | 31.43 |
| ATOM | 1129 | N   | GLN A | 144 | -3.699 | 85.596 | -8.219  | 1.00 | 30.46 |
| ATOM | 1130 | CA  | GLN A | 144 | -4.843 | 84.725 | -8.392  | 1.00 | 28.86 |
| ATOM | 1131 | CB  | GLN A | 144 | -5.275 | 84.696 | -9.858  | 1.00 | 38.80 |
| ATOM | 1132 | CG  | GLN A | 144 | -6.529 | 83.852 | -10.139 | 1.00 | 58.07 |
| ATOM | 1133 | CD  | GLN A | 144 | -7.754 | 84.269 | -9.309  | 1.00 | 67.99 |
| ATOM | 1134 | OE1 | GLN A | 144 | -8.542 | 83.420 | -8.876  | 1.00 | 72.49 |
| ATOM | 1135 | NE2 | GLN A | 144 | -7.922 | 85.573 | -9.099  | 1.00 | 74.56 |
| ATOM | 1136 | C   | GLN A | 144 | -4.449 | 83.339 | -7.938  | 1.00 | 25.81 |
| ATOM | 1137 | O   | GLN A | 144 | -5.201 | 82.669 | -7.239  | 1.00 | 30.61 |
| ATOM | 1138 | N   | TYR A | 145 | -3.259 | 82.905 | -8.335  | 1.00 | 26.62 |
| ATOM | 1139 | CA  | TYR A | 145 | -2.788 | 81.590 | -7.944  | 1.00 | 22.39 |
| ATOM | 1140 | CB  | TYR A | 145 | -1.393 | 81.286 | -8.505  | 1.00 | 21.02 |
| ATOM | 1141 | CG  | TYR A | 145 | -0.895 | 79.930 | -8.047  | 1.00 | 23.34 |
| ATOM | 1142 | CD1 | TYR A | 145 | -1.603 | 78.770 | -8.356  | 1.00 | 21.49 |
| ATOM | 1143 | CE1 | TYR A | 145 | -1.224 | 77.533 | -7.846  | 1.00 | 19.67 |
| ATOM | 1144 | CD2 | TYR A | 145 | 0.221  | 79.814 | -7.219  | 1.00 | 23.57 |
| ATOM | 1145 | CE2 | TYR A | 145 | 0.607  | 78.579 | -6.705  | 1.00 | 20.74 |
| ATOM | 1146 | CZ  | TYR A | 145 | -0.122 | 77.449 | -7.024  | 1.00 | 20.82 |
| ATOM | 1147 | OH  | TYR A | 145 | 0.250  | 76.231 | -6.518  | 1.00 | 24.24 |
| ATOM | 1148 | C   | TYR A | 145 | -2.791 | 81.487 | -6.422  | 1.00 | 22.08 |
| ATOM | 1149 | O   | TYR A | 145 | -3.231 | 80.482 | -5.875  | 1.00 | 24.79 |
| ATOM | 1150 | N   | TYR A | 146 | -2.360 | 82.546 | -5.740  | 1.00 | 20.10 |
| ATOM | 1151 | CA  | TYR A | 146 | -2.329 | 82.552 | -4.283  | 1.00 | 16.74 |
| ATOM | 1152 | CB  | TYR A | 146 | -1.933 | 83.931 | -3.773  | 1.00 | 15.16 |
| ATOM | 1153 | CG  | TYR A | 146 | -1.652 | 83.991 | -2.289  | 1.00 | 19.44 |
| ATOM | 1154 | CD1 | TYR A | 146 | -0.345 | 84.050 | -1.807  | 1.00 | 19.08 |
| ATOM | 1155 | CE1 | TYR A | 146 | -0.088 | 84.132 | -0.458  | 1.00 | 17.67 |
| ATOM | 1156 | CD2 | TYR A | 146 | -2.691 | 84.023 | -1.364  | 1.00 | 18.53 |
| ATOM | 1157 | CE2 | TYR A | 146 | -2.438 | 84.103 | -0.002  | 1.00 | 17.70 |
| ATOM | 1158 | CZ  | TYR A | 146 | -1.137 | 84.161 | 0.437   | 1.00 | 19.52 |
| ATOM | 1159 | OH  | TYR A | 146 | -0.875 | 84.226 | 1.774   | 1.00 | 25.01 |
| ATOM | 1160 | C   | TYR A | 146 | -3.704 | 82.193 | -3.770  | 1.00 | 17.31 |
| ATOM | 1161 | O   | TYR A | 146 | -3.859 | 81.274 | -2.967  | 1.00 | 21.09 |
| ATOM | 1162 | N   | TRP A | 147 | -4.713 | 82.882 | -4.284  | 1.00 | 17.15 |
| ATOM | 1163 | CA  | TRP A | 147 | -6.087 | 82.620 | -3.881  | 1.00 | 17.97 |
| ATOM | 1164 | CB  | TRP A | 147 | -6.988 | 83.752 | -4.363  | 1.00 | 14.43 |

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|      |      |     |       |     |         |        |        |      |       |
|------|------|-----|-------|-----|---------|--------|--------|------|-------|
| ATOM | 1165 | CG  | TRP A | 147 | -6.580  | 85.045 | -3.742 | 1.00 | 16.44 |
| ATOM | 1166 | CD2 | TRP A | 147 | -6.371  | 85.292 | -2.353 | 1.00 | 15.61 |
| ATOM | 1167 | CE2 | TRP A | 147 | -5.855  | 86.588 | -2.222 | 1.00 | 13.55 |
| ATOM | 1168 | CE3 | TRP A | 147 | -6.556  | 84.520 | -1.195 | 1.00 | 13.91 |
| ATOM | 1169 | CD1 | TRP A | 147 | -6.209  | 86.192 | -4.389 | 1.00 | 17.35 |
| ATOM | 1170 | NE1 | TRP A | 147 | -5.760  | 87.122 | -3.482 | 1.00 | 16.82 |
| ATOM | 1171 | CZ2 | TRP A | 147 | -5.526  | 87.138 | -0.999 | 1.00 | 15.71 |
| ATOM | 1172 | CZ3 | TRP A | 147 | -6.225  | 85.066 | 0.023  | 1.00 | 13.54 |
| ATOM | 1173 | CH2 | TRP A | 147 | -5.714  | 86.365 | 0.114  | 1.00 | 14.81 |
| ATOM | 1174 | C   | TRP A | 147 | -6.589  | 81.238 | -4.308 | 1.00 | 19.27 |
| ATOM | 1175 | O   | TRP A | 147 | -7.401  | 80.620 | -3.611 | 1.00 | 19.35 |
| ATOM | 1176 | N   | ASP A | 148 | -6.059  | 80.731 | -5.416 | 1.00 | 18.47 |
| ATOM | 1177 | CA  | ASP A | 148 | -6.416  | 79.405 | -5.904 | 1.00 | 19.12 |
| ATOM | 1178 | CB  | ASP A | 148 | -5.801  | 79.141 | -7.275 | 1.00 | 24.71 |
| ATOM | 1179 | CG  | ASP A | 148 | -6.709  | 79.536 | -8.404 | 1.00 | 26.35 |
| ATOM | 1180 | OD1 | ASP A | 148 | -7.852  | 79.946 | -8.136 | 1.00 | 32.40 |
| ATOM | 1181 | OD2 | ASP A | 148 | -6.284  | 79.423 | -9.569 | 1.00 | 32.06 |
| ATOM | 1182 | C   | ASP A | 148 | -5.973  | 78.328 | -4.927 | 1.00 | 18.33 |
| ATOM | 1183 | O   | ASP A | 148 | -6.797  | 77.536 | -4.486 | 1.00 | 23.56 |
| ATOM | 1184 | N   | VAL A | 149 | -4.679  | 78.276 | -4.603 | 1.00 | 18.47 |
| ATOM | 1185 | CA  | VAL A | 149 | -4.193  | 77.281 | -3.647 | 1.00 | 15.91 |
| ATOM | 1186 | CB  | VAL A | 149 | -2.678  | 77.225 | -3.513 | 1.00 | 14.54 |
| ATOM | 1187 | CG1 | VAL A | 149 | -2.136  | 76.214 | -4.447 | 1.00 | 17.43 |
| ATOM | 1188 | CG2 | VAL A | 149 | -2.055  | 78.590 | -3.729 | 1.00 | 16.13 |
| ATOM | 1189 | C   | VAL A | 149 | -4.757  | 77.549 | -2.271 | 1.00 | 18.11 |
| ATOM | 1190 | O   | VAL A | 149 | -4.897  | 76.633 | -1.467 | 1.00 | 21.98 |
| ATOM | 1191 | N   | PHE A | 150 | -5.032  | 78.814 | -1.979 | 1.00 | 20.18 |
| ATOM | 1192 | CA  | PHE A | 150 | -5.629  | 79.173 | -0.703 | 1.00 | 21.84 |
| ATOM | 1193 | CB  | PHE A | 150 | -5.931  | 80.666 | -0.669 | 1.00 | 19.11 |
| ATOM | 1194 | CG  | PHE A | 150 | -6.441  | 81.152 | 0.651  | 1.00 | 22.86 |
| ATOM | 1195 | CD1 | PHE A | 150 | -5.572  | 81.689 | 1.586  | 1.00 | 22.65 |
| ATOM | 1196 | CD2 | PHE A | 150 | -7.794  | 81.091 | 0.955  | 1.00 | 26.06 |
| ATOM | 1197 | CE1 | PHE A | 150 | -6.045  | 82.158 | 2.800  | 1.00 | 26.82 |
| ATOM | 1198 | CE2 | PHE A | 150 | -8.274  | 81.561 | 2.171  | 1.00 | 22.46 |
| ATOM | 1199 | CZ  | PHE A | 150 | -7.400  | 82.093 | 3.091  | 1.00 | 25.45 |
| ATOM | 1200 | C   | PHE A | 150 | -6.933  | 78.382 | -0.581 | 1.00 | 24.16 |
| ATOM | 1201 | O   | PHE A | 150 | -7.214  | 77.769 | 0.453  | 1.00 | 28.22 |
| ATOM | 1202 | N   | GLY A | 151 | -7.715  | 78.379 | -1.656 | 1.00 | 22.56 |
| ATOM | 1203 | CA  | GLY A | 151 | -8.970  | 77.659 | -1.656 | 1.00 | 20.54 |
| ATOM | 1204 | C   | GLY A | 151 | -8.761  | 76.182 | -1.417 | 1.00 | 21.70 |
| ATOM | 1205 | O   | GLY A | 151 | -9.504  | 75.565 | -0.654 | 1.00 | 25.57 |
| ATOM | 1206 | N   | LEU A | 152 | -7.745  | 75.610 | -2.049 | 1.00 | 18.26 |
| ATOM | 1207 | CA  | LEU A | 152 | -7.460  | 74.193 | -1.876 | 1.00 | 19.08 |
| ATOM | 1208 | CB  | LEU A | 152 | -6.304  | 73.770 | -2.782 | 1.00 | 19.81 |
| ATOM | 1209 | CG  | LEU A | 152 | -5.838  | 72.318 | -2.680 | 1.00 | 19.38 |
| ATOM | 1210 | CD1 | LEU A | 152 | -6.969  | 71.381 | -3.103 | 1.00 | 16.96 |
| ATOM | 1211 | CD2 | LEU A | 152 | -4.615  | 72.127 | -3.538 | 1.00 | 11.13 |
| ATOM | 1212 | C   | LEU A | 152 | -7.093  | 73.916 | -0.425 | 1.00 | 24.24 |
| ATOM | 1213 | O   | LEU A | 152 | -7.667  | 73.032 | 0.219  | 1.00 | 26.47 |
| ATOM | 1214 | N   | SER A | 153 | -6.141  | 74.682 | 0.095  | 1.00 | 24.56 |
| ATOM | 1215 | CA  | SER A | 153 | -5.687  | 74.517 | 1.468  | 1.00 | 22.73 |
| ATOM | 1216 | CB  | SER A | 153 | -4.591  | 75.528 | 1.770  | 1.00 | 21.22 |
| ATOM | 1217 | OG  | SER A | 153 | -3.572  | 75.448 | 0.787  | 1.00 | 21.77 |
| ATOM | 1218 | C   | SER A | 153 | -6.842  | 74.665 | 2.444  | 1.00 | 22.43 |
| ATOM | 1219 | O   | SER A | 153 | -7.041  | 73.823 | 3.316  | 1.00 | 24.75 |
| ATOM | 1220 | N   | SER A | 154 | -7.642  | 75.698 | 2.245  | 1.00 | 22.50 |
| ATOM | 1221 | CA  | SER A | 154 | -8.792  | 75.950 | 3.088  | 1.00 | 25.72 |
| ATOM | 1222 | CB  | SER A | 154 | -9.588  | 77.108 | 2.497  | 1.00 | 25.08 |
| ATOM | 1223 | OG  | SER A | 154 | -10.672 | 77.472 | 3.328  | 1.00 | 38.08 |
| ATOM | 1224 | C   | SER A | 154 | -9.662  | 74.688 | 3.218  | 1.00 | 29.51 |
| ATOM | 1225 | O   | SER A | 154 | -10.140 | 74.356 | 4.310  | 1.00 | 33.28 |
| ATOM | 1226 | N   | ALA A | 155 | -9.786  | 73.941 | 2.121  | 1.00 | 31.53 |
| ATOM | 1227 | CA  | ALA A | 155 | -10.582 | 72.713 | 2.099  | 1.00 | 29.45 |
| ATOM | 1228 | CB  | ALA A | 155 | -11.038 | 72.396 | 0.696  | 1.00 | 30.93 |
| ATOM | 1229 | C   | ALA A | 155 | -9.846  | 71.523 | 2.683  | 1.00 | 28.62 |
| ATOM | 1230 | O   | ALA A | 155 | -10.473 | 70.657 | 3.281  | 1.00 | 32.89 |
| ATOM | 1231 | N   | LEU A | 156 | -8.530  | 71.455 | 2.485  | 1.00 | 28.48 |
| ATOM | 1232 | CA  | LEU A | 156 | -7.739  | 70.355 | 3.032  | 1.00 | 23.61 |
| ATOM | 1233 | CB  | LEU A | 156 | -6.323  | 70.368 | 2.476  | 1.00 | 23.88 |
| ATOM | 1234 | CG  | LEU A | 156 | -6.043  | 69.867 | 1.061  | 1.00 | 20.69 |
| ATOM | 1235 | CD1 | LEU A | 156 | -4.587  | 70.132 | 0.729  | 1.00 | 20.27 |
| ATOM | 1236 | CD2 | LEU A | 156 | -6.325  | 68.394 | 0.958  | 1.00 | 20.84 |
| ATOM | 1237 | C   | LEU A | 156 | -7.688  | 70.488 | 4.547  | 1.00 | 25.37 |

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|      |      |     |       |     |         |        |        |      |       |
|------|------|-----|-------|-----|---------|--------|--------|------|-------|
| ATOM | 1238 | O   | LEU A | 156 | -7.558  | 69.490 | 5.262  | 1.00 | 26.18 |
| ATOM | 1239 | N   | LEU A | 157 | -7.773  | 71.726 | 5.036  | 1.00 | 25.81 |
| ATOM | 1240 | CA  | LEU A | 157 | -7.770  | 71.981 | 6.474  | 1.00 | 25.36 |
| ATOM | 1241 | CB  | LEU A | 157 | -7.557  | 73.466 | 6.775  | 1.00 | 19.73 |
| ATOM | 1242 | CG  | LEU A | 157 | -6.135  | 74.027 | 6.673  | 1.00 | 16.53 |
| ATOM | 1243 | CD1 | LEU A | 157 | -6.111  | 75.418 | 7.270  | 1.00 | 17.68 |
| ATOM | 1244 | CD2 | LEU A | 157 | -5.165  | 73.150 | 7.431  | 1.00 | 15.33 |
| ATOM | 1245 | C   | LEU A | 157 | -9.076  | 71.470 | 7.107  | 1.00 | 29.31 |
| ATOM | 1246 | O   | LEU A | 157 | -9.111  | 71.079 | 8.279  | 1.00 | 32.51 |
| ATOM | 1247 | N   | LYS A | 158 | -10.161 | 71.500 | 6.341  | 1.00 | 33.23 |
| ATOM | 1248 | CA  | LYS A | 158 | -11.442 | 70.982 | 6.814  | 1.00 | 31.84 |
| ATOM | 1249 | CB  | LYS A | 158 | -12.553 | 71.355 | 5.837  | 1.00 | 33.31 |
| ATOM | 1250 | CG  | LYS A | 158 | -12.780 | 72.845 | 5.745  | 1.00 | 34.09 |
| ATOM | 1251 | CD  | LYS A | 158 | -13.850 | 73.167 | 4.738  | 1.00 | 41.31 |
| ATOM | 1252 | CE  | LYS A | 158 | -14.186 | 74.649 | 4.754  | 1.00 | 47.04 |
| ATOM | 1253 | NZ  | LYS A | 158 | -15.362 | 74.923 | 3.886  | 1.00 | 56.43 |
| ATOM | 1254 | C   | LYS A | 158 | -11.289 | 69.460 | 6.905  | 1.00 | 30.71 |
| ATOM | 1255 | O   | LYS A | 158 | -11.770 | 68.836 | 7.848  | 1.00 | 34.49 |
| ATOM | 1256 | N   | GLY A | 159 | -10.570 | 68.884 | 5.942  | 1.00 | 30.71 |
| ATOM | 1257 | CA  | GLY A | 159 | -10.313 | 67.453 | 5.930  | 1.00 | 28.93 |
| ATOM | 1258 | C   | GLY A | 159 | -9.447  | 67.040 | 7.111  | 1.00 | 30.81 |
| ATOM | 1259 | O   | GLY A | 159 | -9.690  | 66.003 | 7.732  | 1.00 | 34.67 |
| ATOM | 1260 | N   | TYR A | 160 | -8.440  | 67.851 | 7.431  | 1.00 | 28.73 |
| ATOM | 1261 | CA  | TYR A | 160 | -7.556  | 67.575 | 8.556  | 1.00 | 29.15 |
| ATOM | 1262 | CB  | TYR A | 160 | -6.378  | 68.554 | 8.556  | 1.00 | 29.86 |
| ATOM | 1263 | CG  | TYR A | 160 | -5.181  | 68.055 | 7.780  | 1.00 | 28.35 |
| ATOM | 1264 | CD1 | TYR A | 160 | -4.828  | 68.607 | 6.543  | 1.00 | 26.01 |
| ATOM | 1265 | CE1 | TYR A | 160 | -3.727  | 68.124 | 5.830  | 1.00 | 25.65 |
| ATOM | 1266 | CD2 | TYR A | 160 | -4.412  | 67.017 | 8.279  | 1.00 | 26.25 |
| ATOM | 1267 | CE2 | TYR A | 160 | -3.321  | 66.530 | 7.584  | 1.00 | 26.20 |
| ATOM | 1268 | CZ  | TYR A | 160 | -2.977  | 67.076 | 6.365  | 1.00 | 28.06 |
| ATOM | 1269 | OH  | TYR A | 160 | -1.884  | 66.546 | 5.711  | 1.00 | 25.91 |
| ATOM | 1270 | C   | TYR A | 160 | -8.313  | 67.646 | 9.884  | 1.00 | 32.18 |
| ATOM | 1271 | O   | TYR A | 160 | -8.034  | 66.884 | 10.812 | 1.00 | 33.45 |
| ATOM | 1272 | N   | ALA A | 161 | -9.262  | 68.571 | 9.976  | 1.00 | 33.22 |
| ATOM | 1273 | CA  | ALA A | 161 | -10.074 | 68.734 | 11.180 | 1.00 | 30.35 |
| ATOM | 1274 | CB  | ALA A | 161 | -10.995 | 69.919 | 11.021 | 1.00 | 30.11 |
| ATOM | 1275 | C   | ALA A | 161 | -10.890 | 67.470 | 11.433 | 1.00 | 31.40 |
| ATOM | 1276 | O   | ALA A | 161 | -10.863 | 66.911 | 12.525 | 1.00 | 32.99 |
| ATOM | 1277 | N   | LEU A | 162 | -11.593 | 67.012 | 10.405 | 1.00 | 30.20 |
| ATOM | 1278 | CA  | LEU A | 162 | -12.405 | 65.813 | 10.501 | 1.00 | 31.99 |
| ATOM | 1279 | CB  | LEU A | 162 | -13.156 | 65.587 | 9.186  | 1.00 | 32.01 |
| ATOM | 1280 | CG  | LEU A | 162 | -14.116 | 66.719 | 8.801  | 1.00 | 33.82 |
| ATOM | 1281 | CD1 | LEU A | 162 | -14.867 | 66.349 | 7.545  | 1.00 | 34.17 |
| ATOM | 1282 | CD2 | LEU A | 162 | -15.096 | 66.997 | 9.933  | 1.00 | 34.51 |
| ATOM | 1283 | C   | LEU A | 162 | -11.580 | 64.580 | 10.877 | 1.00 | 32.42 |
| ATOM | 1284 | O   | LEU A | 162 | -12.002 | 63.767 | 11.696 | 1.00 | 35.19 |
| ATOM | 1285 | N   | ALA A | 163 | -10.396 | 64.453 | 10.291 | 1.00 | 34.99 |
| ATOM | 1286 | CA  | ALA A | 163 | -9.504  | 63.325 | 10.573 | 1.00 | 32.51 |
| ATOM | 1287 | CB  | ALA A | 163 | -8.289  | 63.395 | 9.670  | 1.00 | 28.78 |
| ATOM | 1288 | C   | ALA A | 163 | -9.061  | 63.273 | 12.038 | 1.00 | 30.64 |
| ATOM | 1289 | O   | ALA A | 163 | -8.745  | 62.217 | 12.571 | 1.00 | 30.60 |
| ATOM | 1290 | N   | LEU A | 164 | -8.995  | 64.428 | 12.674 | 1.00 | 29.60 |
| ATOM | 1291 | CA  | LEU A | 164 | -8.578  | 64.478 | 14.054 | 1.00 | 30.80 |
| ATOM | 1292 | CB  | LEU A | 164 | -7.639  | 65.666 | 14.274 | 1.00 | 30.81 |
| ATOM | 1293 | CG  | LEU A | 164 | -6.284  | 65.550 | 13.570 | 1.00 | 29.00 |
| ATOM | 1294 | CD1 | LEU A | 164 | -5.583  | 66.875 | 13.576 | 1.00 | 30.09 |
| ATOM | 1295 | CD2 | LEU A | 164 | -5.434  | 64.509 | 14.245 | 1.00 | 28.45 |
| ATOM | 1296 | C   | LEU A | 164 | -9.778  | 64.529 | 14.993 | 1.00 | 34.67 |
| ATOM | 1297 | O   | LEU A | 164 | -9.633  | 64.811 | 16.179 | 1.00 | 37.15 |
| ATOM | 1298 | N   | GLY A | 165 | -10.964 | 64.258 | 14.455 | 1.00 | 35.40 |
| ATOM | 1299 | CA  | GLY A | 165 | -12.172 | 64.258 | 15.265 | 1.00 | 34.11 |
| ATOM | 1300 | C   | GLY A | 165 | -12.637 | 65.606 | 15.781 | 1.00 | 35.01 |
| ATOM | 1301 | O   | GLY A | 165 | -13.465 | 65.680 | 16.694 | 1.00 | 38.99 |
| ATOM | 1302 | N   | LYS A | 166 | -12.111 | 66.678 | 15.208 | 1.00 | 34.42 |
| ATOM | 1303 | CA  | LYS A | 166 | -12.490 | 68.021 | 15.619 | 1.00 | 34.45 |
| ATOM | 1304 | CB  | LYS A | 166 | -11.267 | 68.924 | 15.571 | 1.00 | 31.93 |
| ATOM | 1305 | CG  | LYS A | 166 | -10.232 | 68.560 | 16.594 | 1.00 | 32.57 |
| ATOM | 1306 | CD  | LYS A | 166 | -10.711 | 68.973 | 17.956 | 1.00 | 34.75 |
| ATOM | 1307 | CE  | LYS A | 166 | -9.756  | 68.522 | 19.022 | 1.00 | 38.74 |
| ATOM | 1308 | NZ  | LYS A | 166 | -10.078 | 69.161 | 20.313 | 1.00 | 40.84 |
| ATOM | 1309 | C   | LYS A | 166 | -13.557 | 68.535 | 14.666 | 1.00 | 37.47 |
| ATOM | 1310 | O   | LYS A | 166 | -13.825 | 67.901 | 13.642 | 1.00 | 41.52 |

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|      |      |     |       |     |         |        |        |      |       |
|------|------|-----|-------|-----|---------|--------|--------|------|-------|
| ATOM | 1311 | N   | GLU A | 167 | -14.189 | 69.660 | 14.994 | 1.00 | 38.98 |
| ATOM | 1312 | CA  | GLU A | 167 | -15.202 | 70.205 | 14.094 | 1.00 | 41.09 |
| ATOM | 1313 | CB  | GLU A | 167 | -15.947 | 71.398 | 14.713 | 1.00 | 45.19 |
| ATOM | 1314 | CG  | GLU A | 167 | -15.110 | 72.638 | 15.025 | 1.00 | 55.15 |
| ATOM | 1315 | CD  | GLU A | 167 | -14.565 | 72.661 | 16.448 | 1.00 | 61.94 |
| ATOM | 1316 | OE1 | GLU A | 167 | -14.118 | 73.742 | 16.887 | 1.00 | 62.92 |
| ATOM | 1317 | OE2 | GLU A | 167 | -14.584 | 71.611 | 17.131 | 1.00 | 64.60 |
| ATOM | 1318 | C   | GLU A | 167 | -14.525 | 70.605 | 12.780 | 1.00 | 41.39 |
| ATOM | 1319 | O   | GLU A | 167 | -13.339 | 70.935 | 12.761 | 1.00 | 41.98 |
| ATOM | 1320 | N   | GLU A | 168 | -15.285 | 70.581 | 11.692 | 1.00 | 39.45 |
| ATOM | 1321 | CA  | GLU A | 168 | -t4.779 | 70.918 | 10.365 | 1.00 | 38.77 |
| ATOM | 1322 | CB  | GLU A | 168 | -15.943 | 70.959 | 9.387  | 1.00 | 40.01 |
| ATOM | 1323 | CG  | GLU A | 168 | -15.535 | 70.844 | 7.951  | 1.00 | 42.60 |
| ATOM | 1324 | CD  | GLU A | 168 | -16.721 | 70.635 | 7.056  | 1.00 | 45.09 |
| ATOM | 1325 | OE1 | GLU A | 168 | -17.408 | 71.626 | 6.740  | 1.00 | 51.44 |
| ATOM | 1326 | OE2 | GLU A | 168 | -16.979 | 69.477 | 6.677  | 1.00 | 50.69 |
| ATOM | 1327 | C   | GLU A | 168 | -13.965 | 72.212 | 10.255 | 1.00 | 37.65 |
| ATOM | 1328 | O   | GLU A | 168 | -12.966 | 72.270 | 9.533  | 1.00 | 37.39 |
| ATOM | 1329 | N   | ASN A | 169 | -14.389 | 73.247 | 10.965 | 1.00 | 34.88 |
| ATOM | 1330 | CA  | ASN A | 169 | -13.696 | 74.527 | 10.925 | 1.00 | 31.36 |
| ATOM | 1331 | CB  | ASN A | 169 | -14.710 | 75.654 | 10.976 | 1.00 | 38.29 |
| ATOM | 1332 | CG  | ASN A | 169 | -15.529 | 75.726 | 9.732  | 1.00 | 46.39 |
| ATOM | 1333 | OD1 | ASN A | 169 | -14.993 | 75.919 | 8.646  | 1.00 | 52.41 |
| ATOM | 1334 | ND2 | ASN A | 169 | -16.833 | 75.544 | 9.865  | 1.00 | 52.70 |
| ATOM | 1335 | C   | ASN A | 169 | -12.677 | 74.717 | 12.029 | 1.00 | 29.02 |
| ATOM | 1336 | O   | ASN A | 169 | -12.264 | 75.839 | 12.318 | 1.00 | 25.13 |
| ATOM | 1337 | N   | PHE A | 170 | -12.236 | 73.618 | 12.617 | 1.00 | 29.52 |
| ATOM | 1338 | CA  | PHE A | 170 | -11.276 | 73.687 | 13.702 | 1.00 | 30.89 |
| ATOM | 1339 | CB  | PHE A | 170 | -10.938 | 72.275 | 14.191 | 1.00 | 34.08 |
| ATOM | 1340 | CG  | PHE A | 170 | -10.030 | 72.248 | 15.377 | 1.00 | 38.01 |
| ATOM | 1341 | CD1 | PHE A | 170 | -10.418 | 72.827 | 16.575 | 1.00 | 41.53 |
| ATOM | 1342 | CD2 | PHE A | 170 | -8.778  | 71.658 | 15.293 | 1.00 | 39.11 |
| ATOM | 1343 | CE1 | PHE A | 170 | -9.571  | 72.824 | 17.675 | 1.00 | 40.36 |
| ATOM | 1344 | CE2 | PHE A | 170 | -7.925  | 71.649 | 16.385 | 1.00 | 41.21 |
| ATOM | 1345 | CZ  | PHE A | 170 | -8.326  | 72.235 | 17.580 | 1.00 | 42.47 |
| ATOM | 1346 | C   | PHE A | 170 | -10.012 | 74.464 | 13.305 | 1.00 | 32.24 |
| ATOM | 1347 | O   | PHE A | 170 | -9.496  | 75.255 | 14.102 | 1.00 | 32.82 |
| ATOM | 1348 | N   | PHE A | 171 | -9.537  | 74.269 | 12.072 | 1.00 | 30.18 |
| ATOM | 1349 | CA  | PHE A | 171 | -8.338  | 74.959 | 11.595 | 1.00 | 25.80 |
| ATOM | 1350 | CB  | PHE A | 171 | -7.436  | 74.018 | 10.780 | 1.00 | 21.23 |
| ATOM | 1351 | CG  | PHE A | 171 | -6.801  | 72.922 | 11.584 | 1.00 | 17.74 |
| ATOM | 1352 | CD1 | PHE A | 171 | -6.984  | 71.592 | 11.232 | 1.00 | 19.14 |
| ATOM | 1353 | CD2 | PHE A | 171 | -6.028  | 73.212 | 12.699 | 1.00 | 20.58 |
| ATOM | 1354 | CE1 | PHE A | 171 | -6.409  | 70.559 | 11.986 | 1.00 | 19.44 |
| ATOM | 1355 | CE2 | PHE A | 171 | -5.449  | 72.188 | 13.457 | 1.00 | 19.74 |
| ATOM | 1356 | CZ  | PHE A | 171 | -5.644  | 70.861 | 13.095 | 1.00 | 18.77 |
| ATOM | 1357 | C   | PHE A | 171 | -8.720  | 76.142 | 10.722 | 1.00 | 27.98 |
| ATOM | 1358 | O   | PHE A | 171 | -8.301  | 77.282 | 10.968 | 1.00 | 26.96 |
| ATOM | 1359 | N   | ALA A | 172 | -9.573  | 75.874 | 9.737  | 1.00 | 27.10 |
| ATOM | 1360 | Q   | ALA A | 172 | -10.009 | 76.880 | 8.770  | 1.00 | 23.60 |
| ATOM | 1361 | CB  | ALA A | 172 | -10.996 | 76.276 | 7.798  | 1.00 | 20.83 |
| ATOM | 1362 | C   | ALA A | 172 | -10.542 | 78.191 | 9.310  | 1.00 | 25.20 |
| ATOM | 1363 | O   | ALA A | 172 | -10.477 | 79.204 | 8.623  | 1.00 | 27.68 |
| ATOM | 1364 | N   | ARG A | 173 | -11.044 | 78.195 | 10.540 | 1.00 | 27.56 |
| ATOM | 1365 | CA  | MG A  | 173 | -11.573 | 79.429 | 11.098 | 1.00 | 28.04 |
| ATOM | 1366 | CB  | ARG A | 173 | -12.374 | 79.170 | 12.377 | 1.00 | 29.47 |
| ATOM | 1367 | CG  | ARG A | 173 | -11.559 | 79.001 | 13.633 | 1.00 | 35.23 |
| ATOM | 1368 | CD  | MG A  | 173 | -12.452 | 78.858 | 14.868 | 1.00 | 40.18 |
| ATOM | 1369 | NE  | MG A  | 173 | -12.898 | 77.482 | 15.106 | 1.00 | 44.83 |
| ATOM | 1370 | CZ  | ARG A | 173 | -14.162 | 77.074 | 15.017 | 1.00 | 48.14 |
| ATOM | 1371 | NH1 | MG A  | 173 | -15.122 | 77.934 | 14.695 | 1.00 | 48.64 |
| ATOM | 1372 | NH2 | MG A  | 173 | -14.468 | 75.800 | 15.240 | 1.00 | 44.20 |
| ATOM | 1373 | C   | MG A  | 173 | -10.433 | 80.401 | 11.355 | 1.00 | 30.23 |
| ATOM | 1374 | O   | ARG A | 173 | -10.657 | 81.591 | 11.584 | 1.00 | 32.24 |
| ATOM | 1375 | N   | HIS A | 174 | -9.206  | 79.889 | 11.314 | 1.00 | 28.30 |
| ATOM | 1376 | CA  | HIS A | 174 | -8.023  | 80.713 | 11.537 | 1.00 | 28.03 |
| ATOM | 1377 | CB  | HIS A | 174 | -7.051  | 79.999 | 12.473 | 1.00 | 25.87 |
| ATOM | 1378 | CG  | HIS A | 174 | -7.622  | 79.688 | 13.816 | 1.00 | 26.33 |
| ATOM | 1379 | CD2 | HIS A | 174 | -8.121  | 78.536 | 14.326 | 1.00 | 28.81 |
| ATOM | 1380 | ND1 | HIS A | 174 | -7.705  | 80.623 | 14.826 | 1.00 | 27.96 |
| ATOM | 1381 | CE1 | HIS A | 174 | -8.228  | 80.059 | 15.900 | 1.00 | 28.08 |
| ATOM | 1382 | NE2 | HIS A | 174 | -8.488  | 78.793 | 15.624 | 1.00 | 27.09 |
| ATOM | 1383 | C   | HIS A | 174 | -7.305  | 81.064 | 10.235 | 1.00 | 27.63 |

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|      |      |     |       |     |         |        |        |      |       |
|------|------|-----|-------|-----|---------|--------|--------|------|-------|
| ATOM | 1384 | O   | HIS A | 174 | -6.371  | 81.865 | 10.240 | 1.00 | 31.26 |
| ATOM | 1385 | N   | PHE A | 175 | -7.734  | 80.442 | 9.138  | 1.00 | 26.90 |
| ATOM | 1386 | CA  | PHE A | 175 | -7.165  | 80.631 | 7.801  | 1.00 | 22.15 |
| ATOM | 1387 | CB  | PHE A | 175 | -7.222  | 79.289 | 7.074  | 1.00 | 21.26 |
| ATOM | 1388 | CG  | PHE A | 175 | -6.293  | 79.176 | 5.911  | 1.00 | 23.40 |
| ATOM | 1389 | CD1 | PHE A | 175 | -6.652  | 78.420 | 4.803  | 1.00 | 20.93 |
| ATOM | 1390 | CD2 | PHE A | 175 | -5.046  | 79.781 | 5.931  | 1.00 | 19.53 |
| ATOM | 1391 | CE1 | PHE A | 175 | -5.789  | 78.266 | 3.741  | 1.00 | 19.79 |
| ATOM | 1392 | CE2 | PHE A | 175 | -4.170  | 79.630 | 4.866  | 1.00 | 19.63 |
| ATOM | 1393 | CZ  | PHE A | 175 | -4.545  | 78.870 | 3.770  | 1.00 | 19.09 |
| ATOM | 1394 | C   | PHE A | 175 | -8.030  | 81.655 | 7.071  | 1.00 | 23.58 |
| ATOM | 1395 | O   | PHE A | 175 | -9.032  | 81.299 | 6.443  | 1.00 | 25.37 |
| ATOM | 1396 | N   | LYS A | 176 | -7.636  | 82.923 | 7.136  | 1.00 | 22.96 |
| ATOM | 1397 | CA  | LYS A | 176 | -8.412  | 84.004 | 6.529  | 1.00 | 26.79 |
| ATOM | 1398 | CB  | LYS A | 176 | -8.991  | 84.922 | 7.619  | 1.00 | 32.23 |
| ATOM | 1399 | CG  | LYS A | 176 | -9.711  | 84.185 | 8.752  | 1.00 | 37.22 |
| ATOM | 1400 | CD  | LYS A | 176 | -10.312 | 85.139 | 9.782  | 1.00 | 45.14 |
| ATOM | 1401 | CE  | LYS A | 176 | -9.271  | 86.065 | 10.408 | 1.00 | 51.76 |
| ATOM | 1402 | NZ  | LYS A | 176 | -8.282  | 85.352 | 11.277 | 1.00 | 54.44 |
| ATOM | 1403 | C   | LYS A | 176 | -7.624  | 84.842 | 5.529  | 1.00 | 26.95 |
| ATOM | 1404 | O   | LYS A | 176 | -6.447  | 85.150 | 5.736  | 1.00 | 29.87 |
| ATOM | 1405 | N   | PRO A | 177 | -8.308  | 85.327 | 4.485  | 1.00 | 24.40 |
| ATOM | 1406 | CD  | PRO A | 177 | -9.714  | 85.067 | 4.146  | 1.00 | 20.13 |
| ATOM | 1407 | CA  | PRO A | 177 | -7.685  | 86.133 | 3.445  | 1.00 | 19.31 |
| ATOM | 1408 | CB  | PRO A | 177 | -8.838  | 86.376 | 2.481  | 1.00 | 16.22 |
| ATOM | 1409 | CG  | PRO A | 177 | -9.687  | 85.187 | 2.664  | 1.00 | 13.22 |
| ATOM | 1410 | C   | PRO A | 177 | -7.084  | 87.434 | 3.903  | 1.00 | 21.14 |
| ATOM | 1411 | O   | PRO A | 177 | -6.096  | 87.883 | 3.349  | 1.00 | 25.46 |
| ATOM | 1412 | N   | ASP A | 178 | -7.660  | 88.049 | 4.917  | 1.00 | 26.69 |
| ATOM | 1413 | CA  | ASP A | 178 | -7.145  | 89.341 | 5.355  | 1.00 | 30.90 |
| ATOM | 1414 | CB  | ASP A | 178 | -8.220  | 90.162 | 6.073  | 1.00 | 40.73 |
| ATOM | 1415 | CG  | ASP A | 178 | -8.927  | 89.377 | 7.153  | 1.00 | 58.65 |
| ATOM | 1416 | OD1 | ASP A | 178 | -9.660  | 88.411 | 6.813  | 1.00 | 67.55 |
| ATOM | 1417 | OD2 | ASP A | 178 | -8.754  | 89.731 | 8.344  | 1.00 | 69.29 |
| ATOM | 1418 | C   | ASP A | 178 | -5.891  | 89.303 | 6.183  | 1.00 | 25.93 |
| ATOM | 1419 | O   | ASP A | 178 | -5.154  | 90.282 | 6.225  | 1.00 | 27.92 |
| ATOM | 1420 | N   | ASP A | 179 | -5.620  | 88.180 | 6.828  | 1.00 | 20.77 |
| ATOM | 1421 | CA  | ASP A | 179 | -4.432  | 88.129 | 7.645  | 1.00 | 20.37 |
| ATOM | 1422 | CB  | ASP A | 179 | -4.790  | 88.332 | 9.120  | 1.00 | 24.28 |
| ATOM | 1423 | CG  | ASP A | 179 | -5.553  | 87.157 | 9.717  | 1.00 | 28.49 |
| ATOM | 1424 | OD1 | ASP A | 179 | -5.957  | 86.249 | 8.967  | 1.00 | 32.76 |
| ATOM | 1425 | OD2 | ASP A | 179 | -5.750  | 87.134 | 10.953 | 1.00 | 34.31 |
| ATOM | 1426 | C   | ASP A | 179 | -3.550  | 86.912 | 7.499  | 1.00 | 20.24 |
| ATOM | 1427 | O   | ASP A | 179 | -2.568  | 86.807 | 8.224  | 1.00 | 22.73 |
| ATOM | 1428 | N   | THR A | 180 | -3.870  | 85.996 | 6.587  | 1.00 | 18.73 |
| ATOM | 1429 | CA  | THR A | 180 | -3.035  | 84.809 | 6.453  | 1.00 | 19.30 |
| ATOM | 1430 | CB  | THR A | 180 | -3.533  | 83.818 | 5.372  | 1.00 | 20.49 |
| ATOM | 1431 | OG1 | THR A | 180 | -2.592  | 82.741 | 5.254  | 1.00 | 20.62 |
| ATOM | 1432 | CG2 | THR A | 180 | -3.657  | 84.488 | 4.024  | 1.00 | 18.20 |
| ATOM | 1433 | C   | THR A | 180 | -1.577  | 85.144 | 6.173  | 1.00 | 22.74 |
| ATOM | 1434 | O   | THR A | 180 | -1.269  | 86.060 | 5.407  | 1.00 | 23.45 |
| ATOM | 1435 | N   | LEU A | 181 | -0.689  | 84.402 | 6.826  | 1.00 | 22.30 |
| ATOM | 1436 | CA  | LEU A | 181 | 0.752   | 84.558 | 6.661  | 1.00 | 19.63 |
| ATOM | 1437 | CB  | LEU A | 181 | 1.450   | 84.460 | 8.023  | 1.00 | 11.22 |
| ATOM | 1438 | CG  | LEU A | 181 | 1.280   | 85.655 | 8.947  | 1.00 | 8.88  |
| ATOM | 1439 | CD1 | LEU A | 181 | 1.760   | 85.318 | 10.332 | 1.00 | 7.59  |
| ATOM | 1440 | CD2 | LEU A | 181 | 2.041   | 86.823 | 8.395  | 1.00 | 9.34  |
| ATOM | 1441 | C   | LEU A | 181 | 1.315   | 83.488 | 5.702  | 1.00 | 19.45 |
| ATOM | 1442 | O   | LEU A | 181 | 2.524   | 83.287 | 5.629  | 1.00 | 22.17 |
| ATOM | 1443 | N   | ALA A | 182 | 0.441   | 82.775 | 5.003  | 1.00 | 15.84 |
| ATOM | 1444 | CA  | ALA A | 182 | 0.886   | 81.749 | 4.072  | 1.00 | 13.71 |
| ATOM | 1445 | CB  | ALA A | 182 | -0.306  | 81.111 | 3.410  | 1.00 | 15.01 |
| ATOM | 1446 | C   | ALA A | 182 | 1.797   | 82.379 | 3.017  | 1.00 | 16.85 |
| ATOM | 1447 | O   | ALA A | 182 | 1.690   | 83.571 | 2.723  | 1.00 | 15.28 |
| ATOM | 1448 | N   | SER A | 183 | 2.679   | 81.583 | 2.429  | 1.00 | 15.86 |
| ATOM | 1449 | CA  | SER A | 183 | 3.584   | 82.108 | 1.416  | 1.00 | 14.12 |
| ATOM | 1450 | CB  | SER A | 183 | 4.947   | 82.430 | 2.039  | 1.00 | 12.59 |
| ATOM | 1451 | OG  | SER A | 183 | 5.585   | 81.250 | 2.497  | 1.00 | 13.59 |
| ATOM | 1452 | C   | SER A | 183 | 3.759   | 81.130 | 0.257  | 1.00 | 13.98 |
| ATOM | 1453 | O   | SER A | 183 | 3.602   | 79.923 | 0.422  | 1.00 | 17.17 |
| ATOM | 1454 | N   | VAL A | 184 | 4.008   | 81.674 | -0.931 | 1.00 | 15.35 |
| ATOM | 1455 | CA  | VAL A | 184 | 4.241   | 80.885 | -2.133 | 1.00 | 13.86 |
| ATOM | 1456 | CB  | VAL A | 184 | 3.366   | 81.361 | -3.335 | 1.00 | 13.35 |

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|      |      |     |       |     |        |        |         |      |       |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 1457 | CG1 | VAL A | 184 | 3.625  | 80.500 | -4.554  | 1.00 | 11.12 |
| ATOM | 1458 | CG2 | VAL A | 184 | 1.907  | 81.283 | -2.994  | 1.00 | 14.34 |
| ATOM | 1459 | C   | VAL A | 184 | 5.698  | 81.161 | -2.479  | 1.00 | 13.94 |
| ATOM | 1460 | O   | VAL A | 184 | 6.123  | 82.314 | -2.459  | 1.00 | 15.07 |
| ATOM | 1461 | N   | VAL A | 185 | 6.469  | 80.107 | -2.722  | 1.00 | 16.12 |
| ATOM | 1462 | CA  | VAL A | 185 | 7.871  | 80.237 | -3.095  | 1.00 | 18.01 |
| ATOM | 1463 | CB  | VAL A | 185 | 8.818  | 79.516 | -2.096  | 1.00 | 19.45 |
| ATOM | 1464 | CG1 | VAL A | 185 | 10.262 | 79.683 | -2.528  | 1.00 | 14.07 |
| ATOM | 1465 | CG2 | VAL A | 185 | 8.629  | 80.054 | -0.708  | 1.00 | 17.49 |
| ATOM | 1466 | C   | VAL A | 185 | 8.039  | 79.551 | -4.438  | 1.00 | 18.98 |
| ATOM | 1467 | O   | VAL A | 185 | 7.660  | 78.391 | -4.585  | 1.00 | 20.19 |
| ATOM | 1468 | N   | LEU A | 186 | 8.541  | 80.282 | -5.428  | 1.00 | 22.23 |
| ATOM | 1469 | CA  | LEU A | 186 | 8.781  | 79.717 | -6.760  | 1.00 | 22.67 |
| ATOM | 1470 | C8  | LEU A | 186 | 8.468  | 80.748 | -7.861  | 1.00 | 17.46 |
| ATOM | 1471 | CG  | LEU A | 186 | 7.117  | 81.480 | -7.844  | 1.00 | 17.76 |
| ATOM | 1472 | CD1 | LEU A | 186 | 6.993  | 82.315 | -9.092  | 1.00 | 19.25 |
| ATOM | 1473 | CD2 | LEU A | 186 | 5.970  | 80.514 | -7.761  | 1.00 | 12.57 |
| ATOM | 1474 | C   | LEU A | 186 | 10.261 | 79.325 | -6.800  | 1.00 | 21.43 |
| ATOM | 1475 | O   | LEU A | 186 | 11.124 | 80.169 | -7.058  | 1.00 | 21.60 |
| ATOM | 1476 | N   | ILE A | 187 | 10.555 | 78.065 | -6.500  | 1.00 | 18.26 |
| ATOM | 1477 | CA  | ILE A | 187 | 11.929 | 77.586 | -6.477  | 1.00 | 18.51 |
| ATOM | 1478 | C8  | ILE A | 187 | 12.068 | 76.373 | -5.547  | 1.00 | 17.33 |
| ATOM | 1479 | CG2 | ILE A | 187 | 13.524 | 75.915 | -5.484  | 1.00 | 17.55 |
| ATOM | 1480 | CG1 | ILE A | 187 | 11.560 | 76.727 | -4.152  | 1.00 | 14.78 |
| ATOM | 1481 | CD1 | ILE A | 187 | 11.608 | 75.582 | -3.201  | 1.00 | 12.56 |
| ATOM | 1482 | C   | ILE A | 187 | 12.421 | 77.183 | -7.858  | 1.00 | 24.55 |
| ATOM | 1483 | O   | ILE A | 187 | 11.688 | 76.567 | -8.632  | 1.00 | 28.10 |
| ATOM | 1484 | N   | ARG A | 188 | 13.671 | 77.509 | -8.158  | 1.00 | 27.00 |
| ATOM | 1485 | CA  | ARG A | 188 | 14.258 | 77.160 | -9.447  | 1.00 | 27.28 |
| ATOM | 1486 | CB  | ARG A | 188 | 14.659 | 78.405 | -10.241 | 1.00 | 25.39 |
| ATOM | 1487 | CG  | ARG A | 188 | 15.481 | 78.037 | -11.466 | 1.00 | 26.11 |
| ATOM | 1488 | CD  | ARG A | 188 | 16.122 | 79.207 | -12.169 | 1.00 | 26.92 |
| ATOM | 1489 | NE  | ARG A | 188 | 16.656 | 78.756 | -13.448 | 1.00 | 33.43 |
| ATOM | 1490 | CZ  | ARG A | 188 | 17.555 | 79.406 | -14.176 | 1.00 | 37.61 |
| ATOM | 1491 | NH1 | M G A | 188 | 18.054 | 80.567 | -13.779 | 1.00 | 40.25 |
| ATOM | 1492 | NH2 | ARG A | 188 | 17.945 | 78.890 | -15.327 | 1.00 | 45.39 |
| ATOM | 1493 | C   | ARG A | 188 | 15.494 | 76.291 | -9.302  | 1.00 | 27.56 |
| ATOM | 1494 | O   | ARG A | 188 | 16.462 | 76.678 | -8.644  | 1.00 | 28.16 |
| ATOM | 1495 | N   | TYR A | 189 | 15.463 | 75.120 | -9.921  | 1.00 | 28.98 |
| ATOM | 1496 | Q   | TYR A | 189 | 16.605 | 74.221 | -9.901  | 1.00 | 30.35 |
| ATOM | 1497 | C8  | TYR A | 189 | 16.166 | 72.799 | -9.600  | 1.00 | 28.57 |
| ATOM | 1498 | CG  | TYR A | 189 | 15.715 | 72.610 | -8.179  | 1.00 | 27.58 |
| ATOM | 1499 | CD1 | TYR A | 189 | 14.363 | 72.586 | -7.862  | 1.00 | 30.42 |
| ATOM | 1500 | CE1 | TYR A | 189 | 13.933 | 72.371 | -6.555  | 1.00 | 32.46 |
| ATOM | 1501 | CD2 | TYR A | 189 | 16.639 | 72.419 | -7.154  | 1.00 | 25.30 |
| ATOM | 1502 | CE2 | TYR A | 189 | 16.224 | 72.206 | -5.846  | 1.00 | 27.43 |
| ATOM | 1503 | CZ  | TYR A | 189 | 14.866 | 72.182 | -5.553  | 1.00 | 31.28 |
| ATOM | 1504 | OH  | TYR A | 189 | 14.434 | 71.980 | -4.262  | 1.00 | 37.45 |
| ATOM | 1505 | C   | TYR A | 189 | 17.225 | 74.335 | -11.293 | 1.00 | 30.75 |
| ATOM | 1506 | O   | TYR A | 189 | 16.643 | 73.905 | -12.278 | 1.00 | 31.49 |
| ATOM | 1507 | N   | PRO A | 190 | 18.396 | 74.974 | -11.388 | 1.00 | 29.84 |
| ATOM | 1508 | CD  | PRO A | 190 | 19.157 | 75.502 | -10.238 | 1.00 | 29.04 |
| ATOM | 1509 | CA  | PRO A | 190 | 19.131 | 75.192 | -12.631 | 1.00 | 29.41 |
| ATOM | 1510 | CB  | PRO A | 190 | 20.122 | 76.271 | -12.222 | 1.00 | 30.04 |
| ATOM | 1511 | CG  | PRO A | 190 | 20.508 | 75.816 | -10.845 | 1.00 | 27.63 |
| ATOM | 1512 | C   | PRO A | 190 | 19.899 | 74.005 | -13.163 | 1.00 | 29.09 |
| ATOM | 1513 | O   | PRO A | 190 | 20.168 | 73.057 | -12.428 | 1.00 | 31.04 |
| ATOM | 1514 | N   | TYR A | 191 | 20.220 | 74.051 | -14.454 | 1.00 | 27.02 |
| ATOM | 1515 | CA  | TYR A | 191 | 21.065 | 73.025 | -15.054 | 1.00 | 25.82 |
| ATOM | 1516 | CB  | TYR A | 191 | 20.612 | 72.611 | -16.449 | 1.00 | 24.40 |
| ATOM | 1517 | CG  | TYR A | 191 | 21.677 | 71.806 | -17.164 | 1.00 | 23.94 |
| ATOM | 1518 | CD1 | TYR A | 191 | 21.959 | 0.497  | -16.779 | 1.00 | 24.85 |
| ATOM | 1519 | CE1 | TYR A | 191 | 22.997 | 69.779 | -17.370 | 1.00 | 26.57 |
| ATOM | 1520 | CD2 | TYR A | 191 | 22.463 | 72.381 | -18.169 | 1.00 | 24.25 |
| ATOM | 1521 | CE2 | TYR A | 191 | 23.509 | 71.674 | -18.764 | 1.00 | 22.72 |
| ATOM | 1522 | CZ  | TYR A | 191 | 23.769 | 70.372 | -18.359 | 1.00 | 27.36 |
| ATOM | 1523 | OH  | TYR A | 191 | 24.791 | 69.655 | -18.938 | 1.00 | 32.34 |
| ATOM | 1524 | C   | TYR A | 191 | 22.406 | 73.737 | -15.167 | 1.00 | 26.75 |
| ATOM | 1525 | O   | TYR A | 191 | 22.477 | 74.848 | -15.697 | 1.00 | 26.19 |
| ATOM | 1526 | N   | LEU A | 192 | 23.453 | 73.131 | -14.620 | 1.00 | 27.75 |
| ATOM | 1527 | CA  | LEU A | 192 | 24.789 | 73.714 | -14.662 | 1.00 | 30.44 |
| ATOM | 1528 | C8  | LEU A | 192 | 25.134 | 74.378 | -13.322 | 1.00 | 27.32 |
| ATOM | 1529 | CG  | LEU A | 192 | 24.221 | 75.486 | -12.789 | 1.00 | 24.54 |

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|      |      |     |       |     |        |        |         |      |       |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 1530 | CD1 | LEU A | 192 | 24.644 | 75.909 | -11.386 | 1.00 | 20.65 |
| ATOM | 1531 | CD2 | LEU A | 192 | 24.252 | 76.664 | -13.738 | 1.00 | 21.14 |
| ATOM | 1532 | C   | LEU A | 192 | 25.856 | 72.673 | -15.013 | 1.00 | 34.74 |
| ATOM | 1533 | O   | LEU A | 192 | 25.803 | 71.511 | -14.586 | 1.00 | 33.09 |
| ATOM | 1534 | N   | ASP A | 193 | 26.778 | 73.085 | -15.867 | 1.00 | 36.86 |
| ATOM | 1535 | CA  | ASP A | 193 | 27.877 | 72.250 | -16.289 | 1.00 | 42.70 |
| ATOM | 1536 | CB  | ASP A | 193 | 27.564 | 71.544 | -17.600 | 1.00 | 48.25 |
| ATOM | 1537 | CG  | ASP A | 193 | 28.732 | 70.728 | -18.106 | 1.00 | 52.17 |
| ATOM | 1538 | OD1 | ASP A | 193 | 29.125 | 70.928 | -19.271 | 1.00 | 58.38 |
| ATOM | 1539 | OD2 | ASP A | 193 | 29.266 | 69.897 | -17.338 | 1.00 | 53.48 |
| ATOM | 1540 | C   | ASP A | 193 | 29.032 | 73.196 | -16.494 | 1.00 | 42.38 |
| ATOM | 1541 | O   | ASP A | 193 | 29.061 | 73.951 | -17.461 | 1.00 | 46.89 |
| ATOM | 1542 | N   | PRO A | 194 | 29.994 | 73.178 | -15.574 | 1.00 | 40.26 |
| ATOM | 1543 | CD  | PRO A | 194 | 31.206 | 74.016 | -15.565 | 1.00 | 40.20 |
| ATOM | 1544 | CA  | PRO A | 194 | 29.956 | 72.294 | -14.414 | 1.00 | 38.87 |
| ATOM | 1545 | CB  | PRO A | 194 | 31.419 | 72.224 | -14.018 | 1.00 | 39.32 |
| ATOM | 1546 | CG  | PRO A | 194 | 31.863 | 73.644 | -14.250 | 1.00 | 39.54 |
| ATOM | 1547 | C   | PRO A | 194 | 29.082 | 72.863 | -13.293 | 1.00 | 40.57 |
| ATOM | 1548 | O   | PRO A | 194 | 28.773 | 74.065 | -13.261 | 1.00 | 39.81 |
| ATOM | 1549 | N   | TYR A | 195 | 28.667 | 71.976 | -12.395 | 1.00 | 38.88 |
| ATOM | 1550 | CA  | TYR A | 195 | 27.826 | 72.341 | -11.269 | 1.00 | 35.95 |
| ATOM | 1551 | CB  | TYR A | 195 | 26.869 | 71.187 | -10.933 | 1.00 | 33.96 |
| ATOM | 1552 | CG  | TYR A | 195 | 25.572 | 71.600 | -10.255 | 1.00 | 33.27 |
| ATOM | 1553 | CD1 | TYR A | 195 | 24.390 | 71.688 | -10.984 | 1.00 | 32.32 |
| ATOM | 1554 | CE1 | TYR A | 195 | 23.200 | 72.048 | -10.381 | 1.00 | 31.47 |
| ATOM | 1555 | CD2 | TYR A | 195 | 25.522 | 71.887 | -8.889  | 1.00 | 29.66 |
| ATOM | 1556 | CE2 | TYR A | 195 | 24.330 | 72.249 | -8.276  | 1.00 | 27.38 |
| ATOM | 1557 | CZ  | TYR A | 195 | 23.178 | 72.325 | -9.030  | 1.00 | 27.54 |
| ATOM | 1558 | OH  | TYR A | 195 | 21.996 | 72.665 | -8.436  | 1.00 | 25.96 |
| ATOM | 1559 | C   | TYR A | 195 | 28.726 | 72.624 | -10.072 | 1.00 | 35.66 |
| ATOM | 1560 | O   | TYR A | 195 | 29.616 | 71.832 | -9.748  | 1.00 | 34.39 |
| ATOM | 1561 | N   | PRO A | 196 | 28.505 | 73.762 | -9.402  | 1.00 | 34.12 |
| ATOM | 1562 | CD  | PRO A | 196 | 27.458 | 74.742 | -9.730  | 1.00 | 32.84 |
| ATOM | 1563 | CA  | PRO A | 196 | 29.270 | 74.183 | -8.231  | 1.00 | 34.92 |
| ATOM | 1564 | CB  | PRO A | 196 | 28.472 | 75.377 | -7.735  | 1.00 | 35.33 |
| ATOM | 1565 | CG  | PRO A | 196 | 27.915 | 75.951 | -8.995  | 1.00 | 36.48 |
| ATOM | 1566 | C   | PRO A | 196 | 29.276 | 73.076 | -7.188  | 1.00 | 40.87 |
| ATOM | 1567 | O   | PRO A | 196 | 28.257 | 72.808 | -6.558  | 1.00 | 44.01 |
| ATOM | 1568 | N   | GLU A | 197 | 30.418 | 72.425 | -7.013  | 1.00 | 46.54 |
| ATOM | 1569 | CA  | GLU A | 197 | 30.535 | 71.337 | -6.048  | 1.00 | 49.40 |
| ATOM | 1570 | CB  | GLU A | 197 | 31.992 | 70.896 | -5.916  | 1.00 | 59.62 |
| ATOM | 1571 | CG  | GLU A | 197 | 32.595 | 70.350 | -7.211  | 1.00 | 74.74 |
| ATOM | 1572 | CD  | GLU A | 197 | 34.093 | 70.061 | -7.108  | 1.00 | 82.34 |
| ATOM | 1573 | OE1 | GLU A | 197 | 34.807 | 70.797 | -6.383  | 1.00 | 86.57 |
| ATOM | 1574 | OE2 | GLU A | 197 | 34.558 | 69.100 | -7.765  | 1.00 | 87.43 |
| ATOM | 1575 | C   | GLU A | 197 | 30.007 | 71.757 | -4.692  | 1.00 | 45.50 |
| ATOM | 1576 | O   | GLU A | 197 | 29.395 | 70.972 | -3.985  | 1.00 | 46.60 |
| ATOM | 1577 | N   | ALA A | 198 | 30.216 | 73.018 | -4.352  | 1.00 | 43.56 |
| ATOM | 1578 | CA  | ALA A | 198 | 29.765 | 73.538 | -3.072  | 1.00 | 42.05 |
| ATOM | 1579 | CB  | ALA A | 198 | 30.214 | 74.968 | -2.908  | 1.00 | 42.58 |
| ATOM | 1580 | C   | ALA A | 198 | 28.264 | 73.443 | -2.861  | 1.00 | 41.83 |
| ATOM | 1581 | O   | ALA A | 198 | 27.805 | 73.315 | -1.728  | 1.00 | 46.61 |
| ATOM | 1582 | N   | ALA A | 199 | 27.501 | 73.501 | -3.946  | 1.00 | 36.04 |
| ATOM | 1583 | CA  | ALA A | 199 | 26.052 | 73.450 | -3.852  | 1.00 | 32.51 |
| ATOM | 1584 | CB  | ALA A | 199 | 25.430 | 74.173 | -5.019  | 1.00 | 33.11 |
| ATOM | 1585 | C   | ALA A | 199 | 25.512 | 72.044 | -3.772  | 1.00 | 33.23 |
| ATOM | 1586 | O   | ALA A | 199 | 24.307 | 71.837 | -3.900  | 1.00 | 38.62 |
| ATOM | 1587 | N   | ILE A | 200 | 26.397 | 71.075 | -3.590  | 1.00 | 32.94 |
| ATOM | 1588 | CA  | ILE A | 200 | 25.973 | 69.687 | -3.508  | 1.00 | 34.13 |
| ATOM | 1589 | CB  | ILE A | 200 | 26.565 | 68.846 | -4.644  | 1.00 | 30.62 |
| ATOM | 1590 | CG2 | ILE A | 200 | 26.086 | 67.409 | -4.527  | 1.00 | 19.56 |
| ATOM | 1591 | CG1 | ILE A | 200 | 26.154 | 69.451 | -5.998  | 1.00 | 31.15 |
| ATOM | 1592 | CD1 | ILE A | 200 | 27.065 | 69.109 | -7.124  | 1.00 | 34.14 |
| ATOM | 1593 | C   | ILE A | 200 | 26.353 | 69.073 | -2.182  | 1.00 | 37.98 |
| ATOM | 1594 | O   | ILE A | 200 | 27.525 | 68.817 | -1.909  | 1.00 | 42.30 |
| ATOM | 1595 | N   | LYS A | 201 | 25.343 | 68.844 | -1.356  | 1.00 | 41.21 |
| ATOM | 1596 | CA  | LYS A | 201 | 25.541 | 68.258 | -0.045  | 1.00 | 42.08 |
| ATOM | 1597 | CB  | LYS A | 201 | 24.485 | 68.776 | 0.935   | 1.00 | 44.17 |
| ATOM | 1598 | CG  | LYS A | 201 | 24.592 | 70.275 | 1.203   | 1.00 | 47.76 |
| ATOM | 1599 | CD  | LYS A | 201 | 23.219 | 70.918 | 1.218   | 1.00 | 52.10 |
| ATOM | 1600 | CE  | LYS A | 201 | 23.302 | 72.423 | 1.021   | 1.00 | 52.22 |
| ATOM | 1601 | NZ  | LYS A | 201 | 21.940 | 73.026 | 0.955   | 1.00 | 52.59 |
| ATOM | 1602 | C   | LYS A | 201 | 25.443 | 66.761 | -0.179  | 1.00 | 39.59 |

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|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 1603 | O   | LYS A | 201 | 24.587 | 66.255 | -0.886 | 1.00 | 42.27 |
| ATOM | 1604 | N   | THR A | 202 | 26.338 | 66.052 | 0.485  | 1.00 | 40.47 |
| ATOM | 1605 | CA  | THR A | 202 | 26.329 | 64.605 | 0.424  | 1.00 | 42.05 |
| ATOM | 1606 | CB  | THR A | 202 | 27.682 | 64.062 | -0.114 | 1.00 | 38.96 |
| ATOM | 1607 | OG1 | THR A | 202 | 27.900 | 62.727 | 0.356  | 1.00 | 42.95 |
| ATOM | 1608 | CG2 | THR A | 202 | 28.838 | 64.970 | 0.276  | 1.00 | 40.84 |
| ATOM | 1609 | C   | THR A | 202 | 25.908 | 64.022 | 1.781  | 1.00 | 42.98 |
| ATOM | 1610 | O   | THR A | 202 | 26.553 | 64.247 | 2.809  | 1.00 | 47.33 |
| ATOM | 1611 | N   | ALA A | 203 | 24.750 | 63.369 | 1.785  | 1.00 | 41.07 |
| ATOM | 1612 | CA  | ALA A | 203 | 24.195 | 62.776 | 2.995  | 1.00 | 42.49 |
| ATOM | 1613 | Q   | ALA A | 203 | 22.824 | 62.179 | 2.713  | 1.00 | 36.69 |
| ATOM | 1614 | C   | ALA A | 203 | 25.110 | 61.705 | 3.525  | 1.00 | 44.40 |
| ATOM | 1615 | O   | ALA A | 203 | 25.924 | 61.159 | 2.787  | 1.00 | 45.26 |
| ATOM | 1616 | N   | ALA A | 204 | 24.920 | 61.348 | 4.788  | 1.00 | 47.23 |
| ATOM | 1617 | CA  | ALA A | 204 | 25.733 | 60.316 | 5.408  | 1.00 | 47.81 |
| ATOM | 1618 | Q   | ALA A | 204 | 25.266 | 60.089 | 6.817  | 1.00 | 48.23 |
| ATOM | 1619 | C   | ALA A | 204 | 25.701 | 59.000 | 4.615  | 1.00 | 48.73 |
| ATOM | 1620 | O   | ALA A | 204 | 26.680 | 58.252 | 4.581  | 1.00 | 51.77 |
| ATOM | 1621 | N   | ASP A | 205 | 24.574 | 58.725 | 3.970  | 1.00 | 45.72 |
| ATOM | 1622 | CA  | ASP A | 205 | 24.437 | 57.501 | 3.189  | 1.00 | 42.78 |
| ATOM | 1623 | CB  | ASP A | 205 | 22.984 | 56.989 | 3.221  | 1.00 | 47.36 |
| ATOM | 1624 | CG  | ASP A | 205 | 22.018 | 57.827 | 2.370  | 1.00 | 50.09 |
| ATOM | 1625 | OD1 | ASP A | 205 | 22.374 | 58.937 | 1.922  | 1.00 | 54.80 |
| ATOM | 1626 | OD2 | ASP A | 205 | 20.880 | 57.362 | 2.147  | 1.00 | 48.85 |
| ATOM | 1627 | C   | ASP A | 205 | 24.915 | 57.644 | 1.751  | 1.00 | 39.10 |
| ATOM | 1628 | O   | ASP A | 205 | 24.628 | 56.787 | 0.924  | 1.00 | 39.36 |
| ATOM | 1629 | N   | GLY A | 206 | 25.597 | 58.744 | 1.447  | 1.00 | 37.66 |
| ATOM | 1630 | CA  | GLY A | 206 | 26.100 | 58.968 | 0.097  | 1.00 | 36.43 |
| ATOM | 1631 | C   | GLY A | 206 | 25.238 | 59.669 | -0.950 | 1.00 | 34.15 |
| ATOM | 1632 | O   | GLY A | 206 | 25.739 | 60.024 | -2.017 | 1.00 | 31.94 |
| ATOM | 1633 | N   | THR A | 207 | 23.956 | 59.877 | -0.679 | 1.00 | 29.49 |
| ATOM | 1634 | CA  | THR A | 207 | 23.109 | 60.538 | -1.657 | 1.00 | 25.87 |
| ATOM | 1635 | CB  | THR A | 207 | 21.637 | 60.442 | -1.260 | 1.00 | 27.03 |
| ATOM | 1636 | OG1 | THR A | 207 | 21.345 | 59.109 | -0.824 | 1.00 | 29.78 |
| ATOM | 1637 | CG2 | THR A | 207 | 20.766 | 60.752 | -2.447 | 1.00 | 28.36 |
| ATOM | 1638 | C   | THR A | 207 | 23.509 | 61.998 | -1.837 | 1.00 | 25.47 |
| ATOM | 1639 | O   | THR A | 207 | 23.891 | 62.663 | -0.881 | 1.00 | 27.07 |
| ATOM | 1640 | N   | LYS A | 208 | 23.481 | 62.478 | -3.073 | 1.00 | 26.75 |
| ATOM | 1641 | CA  | LYS A | 208 | 23.828 | 63.866 | -3.347 | 1.00 | 28.57 |
| ATOM | 1642 | Q   | LYS A | 208 | 24.323 | 64.035 | -4.785 | 1.00 | 34.36 |
| ATOM | 1643 | CG  | LYS A | 208 | 25.565 | 63.216 | -5.112 | 1.00 | 40.54 |
| ATOM | 1644 | CD  | LYS A | 208 | 26.734 | 63.592 | -4.210 | 1.00 | 53.48 |
| ATOM | 1645 | CE  | LYS A | 208 | 27.937 | 62.669 | -4.416 | 1.00 | 58.70 |
| ATOM | 1646 | NZ  | LYS A | 208 | 29.114 | 63.071 | -3.586 | 1.00 | 62.46 |
| ATOM | 1647 | C   | LYS A | 208 | 22.540 | 64.626 | -3.124 | 1.00 | 27.85 |
| ATOM | 1648 | O   | LYS A | 208 | 21.497 | 64.231 | -3.638 | 1.00 | 29.27 |
| ATOM | 1649 | N   | LEU A | 209 | 22.620 | 65.743 | -2.413 | 1.00 | 25.63 |
| ATOM | 1650 | CA  | LEU A | 209 | 21.442 | 66.518 | -2.066 | 1.00 | 18.54 |
| ATOM | 1651 | CB  | LEU A | 209 | 21.149 | 66.348 | -0.583 | 1.00 | 15.76 |
| ATOM | 1652 | CG  | LEU A | 209 | 21.027 | 64.949 | -0.009 | 1.00 | 16.54 |
| ATOM | 1653 | CD1 | LEU A | 209 | 21.176 | 65.029 | 1.478  | 1.00 | 19.47 |
| ATOM | 1654 | CD2 | LEU A | 209 | 19.704 | 64.330 | -0.393 | 1.00 | 14.83 |
| ATOM | 1655 | C   | LEU A | 209 | 21.570 | 67.997 | -2.303 | 1.00 | 19.56 |
| ATOM | 1656 | O   | LEU A | 209 | 22.647 | 68.561 | -2.184 | 1.00 | 20.20 |
| ATOM | 1657 | N   | SER A | 210 | 20.438 | 68.624 | -2.591 | 1.00 | 20.72 |
| ATOM | 1658 | CA  | SER A | 210 | 20.359 | 70.064 | -2.782 | 1.00 | 26.32 |
| ATOM | 1659 | CA  | SER A | 210 | 19.243 | 70.433 | -3.770 | 1.00 | 26.58 |
| ATOM | 1660 | OG  | SER A | 210 | 19.611 | 70.186 | -5.115 | 1.00 | 34.59 |
| ATOM | 1661 | C   | SER A | 210 | 20.000 | 70.625 | -1.407 | 1.00 | 26.44 |
| ATOM | 1662 | O   | SER A | 210 | 20.466 | 71.694 | -1.023 | 1.00 | 29.35 |
| ATOM | 1663 | N   | PHE A | 211 | 19.143 | 69.900 | -0.683 | 1.00 | 27.04 |
| ATOM | 1664 | CA  | PHE A | 211 | 18.691 | 70.296 | 0.652  | 1.00 | 24.33 |
| ATOM | 1665 | CB  | PHE A | 211 | 17.306 | 70.938 | 0.603  | 1.00 | 25.32 |
| ATOM | 1666 | CG  | PHE A | 211 | 17.275 | 72.243 | -0.123 | 1.00 | 27.69 |
| ATOM | 1667 | CD1 | PHE A | 211 | 16.682 | 72.341 | -1.378 | 1.00 | 35.01 |
| ATOM | 1668 | CD2 | PHE A | 211 | 17.867 | 73.370 | 0.426  | 1.00 | 31.73 |
| ATOM | 1669 | CE1 | PHE A | 211 | 16.681 | 73.547 | -2.082 | 1.00 | 35.58 |
| ATOM | 1670 | CE2 | PHE A | 211 | 17.875 | 74.586 | -0.269 | 1.00 | 34.04 |
| ATOM | 1671 | CZ  | PHE A | 211 | 17.281 | 74.672 | -1.525 | 1.00 | 36.38 |
| ATOM | 1672 | C   | PHE A | 211 | 18.670 | 69.116 | 1.611  | 1.00 | 24.35 |
| ATOM | 1673 | O   | PHE A | 211 | 18.062 | 68.076 | 1.339  | 1.00 | 21.15 |
| ATOM | 1674 | N   | GLU A | 212 | 19.354 | 69.304 | 2.732  | 1.00 | 25.04 |
| ATOM | 1675 | CA  | GLU A | 212 | 19.485 | 68.311 | 3.777  | 1.00 | 26.00 |

|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 1676 | CB  | GLU A | 212 | 20.580 | 68.763 | 4.742  | 1.00 | 31.89 |
| ATOM | 1677 | CG  | GLU A | 212 | 21.004 | 67.726 | 5.770  | 1.00 | 52.30 |
| ATOM | 1678 | CD  | GLU A | 212 | 21.605 | 66.472 | 5.145  | 1.00 | 60.61 |
| ATOM | 1679 | OE1 | GLU A | 212 | 20.903 | 65.434 | 5.092  | 1.00 | 59.97 |
| ATOM | 1680 | OE2 | GLU A | 212 | 22.786 | 66.527 | 4.718  | 1.00 | 67.14 |
| ATOM | 1681 | C   | GLU A | 212 | 18.158 | 68.100 | 4.500  | 1.00 | 24.80 |
| ATOM | 1682 | O   | GLU A | 212 | 17.243 | 68.918 | 4.392  | 1.00 | 22.54 |
| ATOM | 1683 | N   | TRP A | 213 | 18.059 | 66.997 | 5.234  | 1.00 | 26.64 |
| ATOM | 1684 | CA  | TRP A | 213 | 16.846 | 66.653 | 5.963  | 1.00 | 28.18 |
| ATOM | 1685 | CB  | TRP A | 213 | 17.062 | 65.393 | 6.811  | 1.00 | 27.08 |
| ATOM | 1686 | CG  | TRP A | 213 | 17.942 | 65.589 | 7.993  | 1.00 | 31.90 |
| ATOM | 1687 | CD2 | TRP A | 213 | 17.541 | 66.016 | 9.295  | 1.00 | 34.81 |
| ATOM | 1688 | CE2 | TRP A | 213 | 18.702 | 66.070 | 10.093 | 1.00 | 39.48 |
| ATOM | 1689 | CE3 | TRP A | 213 | 16.310 | 66.353 | 9.867  | 1.00 | 35.14 |
| ATOM | 1690 | CD1 | TRP A | 213 | 19.291 | 65.406 | 8.051  | 1.00 | 34.70 |
| ATOM | 1691 | NE1 | TRP A | 213 | 19.759 | 65.698 | 9.306  | 1.00 | 38.91 |
| ATOM | 1692 | CZ2 | TRP A | 213 | 18.671 | 66.456 | 11.436 | 1.00 | 39.22 |
| ATOM | 1693 | CZ3 | TRP A | 213 | 16.278 | 66.736 | 11.198 | 1.00 | 36.20 |
| ATOM | 1694 | CH2 | TRP A | 213 | 17.452 | 66.780 | 11.969 | 1.00 | 39.04 |
| ATOM | 1695 | C   | TRP A | 213 | 16.312 | 67.780 | 6.840  | 1.00 | 27.32 |
| ATOM | 1696 | O   | TRP A | 213 | 17.074 | 68.601 | 7.341  | 1.00 | 26.78 |
| ATOM | 1697 | N   | HIS A | 214 | 14.994 | 67.785 | 7.033  | 1.00 | 25.99 |
| ATOM | 1698 | CA  | HIS A | 214 | 14.312 | 68.785 | 9.843  | 1.00 | 21.26 |
| ATOM | 1699 | CB  | HIS A | 214 | 14.498 | 70.170 | 7.229  | 1.00 | 24.00 |
| ATOM | 1700 | CG  | HIS A | 214 | 14.011 | 70.268 | 5.815  | 1.00 | 26.31 |
| ATOM | 1701 | CD2 | HIS A | 214 | 12.986 | 70.964 | 5.265  | 1.00 | 20.40 |
| ATOM | 1702 | ND1 | HIS A | 214 | 14.604 | 69.575 | 4.782  | 1.00 | 24.70 |
| ATOM | 1703 | CE1 | HIS A | 214 | 13.966 | 69.840 | 3.657  | 1.00 | 19.84 |
| ATOM | 1704 | NE2 | HIS A | 214 | 12.983 | 70.682 | 3.921  | 1.00 | 19.56 |
| ATOM | 1705 | C   | HIS A | 214 | 12.824 | 68.508 | 7.915  | 1.00 | 20.75 |
| ATOM | 1706 | O   | HIS A | 214 | 12.295 | 67.628 | 7.230  | 1.00 | 22.27 |
| ATOM | 1707 | N   | GLU A | 215 | 12.153 | 69.316 | 8.718  | 1.00 | 21.29 |
| ATOM | 1708 | Q   | GLU A | 215 | 10.710 | 69.258 | 8.888  | 1.00 | 25.72 |
| ATOM | 1709 | CB  | GLU A | 215 | 10.347 | 68.937 | 10.341 | 1.00 | 27.88 |
| ATOM | 1710 | CG  | GLU A | 215 | 11.325 | 69.505 | 11.344 | 1.00 | 44.01 |
| ATOM | 1711 | CD  | GLU A | 215 | 10.962 | 69.188 | 12.773 | 1.00 | 49.99 |
| ATOM | 1712 | OE1 | GLU A | 215 | 10.532 | 68.043 | 13.040 | 1.00 | 48.65 |
| ATOM | 1713 | OE2 | GLU A | 215 | 11.118 | 70.089 | 13.628 | 1.00 | 56.84 |
| ATOM | 1714 | C   | GLU A | 215 | 10.320 | 70.676 | 8.504  | 1.00 | 23.84 |
| ATOM | 1715 | O   | GLU A | 215 | 11.116 | 71.595 | 8.672  | 1.00 | 24.88 |
| ATOM | 1716 | N   | ASP A | 216 | 9.136  | 70.858 | 7.935  | 1.00 | 22.73 |
| ATOM | 1717 | CA  | ASP A | 216 | 8.732  | 72.187 | 7.492  | 1.00 | 22.94 |
| ATOM | 1718 | CB  | ASP A | 216 | 7.636  | 72.112 | 6.407  | 1.00 | 27.97 |
| ATOM | 1719 | CG  | ASP A | 216 | 8.082  | 71.398 | 5.135  | 1.00 | 27.71 |
| ATOM | 1720 | OD1 | ASP A | 216 | 9.304  | 71.232 | 4.918  | 1.00 | 31.88 |
| ATOM | 1721 | OD2 | ASP A | 216 | 7.185  | 71.015 | 4.344  | 1.00 | 26.49 |
| ATOM | 1722 | C   | ASP A | 216 | 8.230  | 73.096 | 8.596  | 1.00 | 19.73 |
| ATOM | 1723 | O   | ASP A | 216 | 7.680  | 72.652 | 9.594  | 1.00 | 23.16 |
| ATOM | 1724 | N   | VAL A | 217 | 8.433  | 74.384 | 8.398  | 1.00 | 16.59 |
| ATOM | 1725 | CA  | VAL A | 217 | 7.945  | 75.376 | 9.312  | 1.00 | 18.55 |
| ATOM | 1726 | CB  | VAL A | 217 | 8.907  | 76.564 | 9.424  | 1.00 | 16.49 |
| ATOM | 1727 | CG1 | VAL A | 217 | 8.265  | 77.687 | 10.235 | 1.00 | 10.45 |
| ATOM | 1728 | CG2 | VAL A | 217 | 10.179 | 76.123 | 10.088 | 1.00 | 11.70 |
| ATOM | 1729 | C   | VAL A | 217 | 6.652  | 75.819 | 8.633  | 1.00 | 23.10 |
| ATOM | 1730 | O   | VAL A | 217 | 6.667  | 76.674 | 7.729  | 1.00 | 21.60 |
| ATOM | 1731 | N   | SER A | 218 | 5.562  | 75.142 | 8.990  | 1.00 | 25.06 |
| ATOM | 1732 | CA  | SER A | 218 | 4.233  | 75.433 | 8.452  | 1.00 | 24.44 |
| ATOM | 1733 | CB  | SER A | 218 | 4.183  | 75.110 | 6.954  | 1.00 | 23.25 |
| ATOM | 1734 | OG  | SER A | 218 | 4.109  | 73.706 | 6.717  | 1.00 | 16.35 |
| ATOM | 1735 | C   | SER A | 218 | 3.190  | 74.585 | 9.178  | 1.00 | 23.44 |
| ATOM | 1736 | O   | SER A | 218 | 3.541  | 73.734 | 9.996  | 1.00 | 23.65 |
| ATOM | 1737 | N   | LEU A | 219 | 1.913  | 74.865 | 8.932  | 1.00 | 21.85 |
| ATOM | 1738 | CA  | LEU A | 219 | 0.847  | 74.064 | 9.518  | 1.00 | 22.52 |
| ATOM | 1739 | CB  | LEU A | 219 | -0.493 | 74.797 | 9.483  | 1.00 | 22.11 |
| ATOM | 1740 | CG  | LEU A | 219 | -1.687 | 73.960 | 9.955  | 1.00 | 18.98 |
| ATOM | 1741 | CD1 | LEU A | 219 | -1.427 | 73.419 | 11.330 | 1.00 | 17.47 |
| ATOM | 1742 | CD2 | LEU A | 219 | -2.933 | 74.804 | 9.956  | 1.00 | 19.86 |
| ATOM | 1743 | C   | LEU A | 219 | 0.822  | 72.817 | 8.633  | 1.00 | 24.74 |
| ATOM | 1744 | O   | LEU A | 219 | 0.870  | 71.697 | 9.128  | 1.00 | 26.48 |
| ATOM | 1745 | N   | ILE A | 220 | 0.760  | 73.030 | 7.318  | 1.00 | 24.79 |
| ATOM | 1746 | CA  | ILE A | 220 | 0.821  | 71.960 | 6.309  | 1.00 | 22.56 |
| ATOM | 1747 | CB  | ILE A | 220 | -0.563 | 71.393 | 5.860  | 1.00 | 21.63 |
| ATOM | 1748 | CG2 | ILE A | 220 | -1.335 | 70.840 | 7.040  | 1.00 | 20.63 |

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|      |      |     |       |     |        |        |         |      |       |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 1749 | CG1 | ILE A | 220 | -1.380 | 72.443 | 5.109   | 1.00 | 22.42 |
| ATOM | 1750 | CD1 | ILE A | 220 | -2.505 | 71.841 | 4.297   | 1.00 | 18.13 |
| ATOM | 1751 | C   | ILE A | 220 | 1.501  | 72.600 | 5.099   | 1.00 | 18.56 |
| ATOM | 1752 | O   | ILE A | 220 | 1.496  | 73.825 | 4.970   | 1.00 | 17.45 |
| ATOM | 1753 | N   | THR A | 221 | 2.141  | 71.793 | 4.263   | 1.00 | 17.74 |
| ATOM | 1754 | CA  | THR A | 221 | 2.802  | 72.295 | 3.069   | 1.00 | 14.91 |
| ATOM | 1755 | CB  | THR A | 221 | 4.287  | 71.939 | 3.032   | 1.00 | 15.95 |
| ATOM | 1756 | OG1 | THR A | 221 | 4.937  | 72.557 | 4.146   | 1.00 | 18.73 |
| ATOM | 1757 | CG2 | THR A | 221 | 4.928  | 72.469 | 1.773   | 1.00 | 10.41 |
| ATOM | 1758 | C   | THR A | 221 | 2.066  | 71.651 | 1.916   | 1.00 | 16.30 |
| ATOM | 1759 | O   | THR A | 221 | 1.711  | 70.477 | 1.983   | 1.00 | 18.87 |
| ATOM | 1760 | N   | VAL A | 222 | 1.729  | 72.477 | 0.933   | 1.00 | 16.62 |
| ATOM | 1761 | CA  | VAL A | 222 | 0.992  | 72.088 | -0.261  | 1.00 | 17.81 |
| ATOM | 1762 | CB  | VAL A | 222 | -0.332 | 72.880 | -0.310  | 1.00 | 22.05 |
| ATOM | 1763 | CG1 | VAL A | 222 | -1.046 | 72.671 | -1.630  | 1.00 | 25.61 |
| ATOM | 1764 | CG2 | VAL A | 222 | -1.221 | 72.446 | 0.854   | 1.00 | 24.18 |
| ATOM | 1765 | C   | VAL A | 222 | 1.890  | 72.404 | -1.464  | 1.00 | 17.84 |
| ATOM | 1766 | O   | VAL A | 222 | 1.990  | 73.557 | -1.895  | 1.00 | 18.42 |
| ATOM | 1767 | N   | LEU A | 223 | 2.525  | 71.359 | -1.995  | 1.00 | 14.96 |
| ATOM | 1768 | CA  | LEU A | 223 | 3.495  | 71.469 | -3.080  | 1.00 | 15.97 |
| ATOM | 1769 | CB  | LEU A | 223 | 4.779  | 70.761 | -2.647  | 1.00 | 8.17  |
| ATOM | 1770 | CG  | LEU A | 223 | 5.836  | 70.407 | -3.680  | 1.00 | 9.19  |
| ATOM | 1771 | CD1 | LEU A | 223 | 6.771  | 71.557 | -3.882  | 1.00 | 9.69  |
| ATOM | 1772 | CD2 | LEU A | 223 | 6.605  | 69.205 | -3.191  | 1.00 | 12.71 |
| ATOM | 1773 | C   | LEU A | 223 | 3.146  | 70.951 | -4.461  | 1.00 | 20.09 |
| ATOM | 1774 | O   | LEU A | 223 | 2.623  | 69.846 | -4.608  | 1.00 | 24.25 |
| ATOM | 1775 | N   | TYR A | 224 | 3.453  | 71.757 | -5.476  | 1.00 | 23.92 |
| ATOM | 1776 | CA  | TYR A | 224 | 3.283  | 71.340 | -6.862  | 1.00 | 22.47 |
| ATOM | 1777 | CB  | TYR A | 224 | 2.415  | 72.269 | -7.711  | 1.00 | 25.33 |
| ATOM | 1778 | CG  | TYR A | 224 | 2.258  | 71.701 | -9.110  | 1.00 | 24.10 |
| ATOM | 1779 | CD1 | TYR A | 224 | 1.592  | 70.488 | -9.311  | 1.00 | 22.12 |
| ATOM | 1780 | CE1 | TYR A | 224 | 1.534  | 69.893 | -10.560 | 1.00 | 25.03 |
| ATOM | 1781 | CD2 | TYR A | 224 | 2.860  | 72.311 | -10.212 | 1.00 | 23.73 |
| ATOM | 1782 | CE2 | TYR A | 224 | 2.811  | 71.720 | -11.475 | 1.00 | 27.76 |
| ATOM | 1783 | CZ  | TYR A | 224 | 2.146  | 70.505 | -11.643 | 1.00 | 29.83 |
| ATOM | 1784 | OH  | TYR A | 224 | 2.112  | 69.895 | -12.884 | 1.00 | 31.58 |
| ATOM | 1785 | C   | TYR A | 224 | 4.680  | 71.314 | -7.451  | 1.00 | 25.24 |
| ATOM | 1786 | O   | TYR A | 224 | 5.424  | 72.301 | -7.392  | 1.00 | 27.50 |
| ATOM | 1787 | N   | GLN A | 225 | 5.014  | 70.193 | -8.060  | 1.00 | 23.63 |
| ATOM | 1788 | CA  | GLN A | 225 | 6.327  | 70.006 | -8.639  | 1.00 | 25.73 |
| ATOM | 1789 | Q   | GLN A | 225 | 7.184  | 69.294 | -7.609  | 1.00 | 23.37 |
| ATOM | 1790 | CG  | GLN A | 225 | 8.614  | 69.292 | -7.891  | 1.00 | 25.23 |
| ATOM | 1791 | CD  | GLN A | 225 | 9.378  | 68.781 | -6.720  | 1.00 | 30.69 |
| ATOM | 1792 | OE1 | GLN A | 225 | 10.264 | 69.461 | -6.203  | 1.00 | 37.77 |
| ATOM | 1793 | NE2 | GLN A | 225 | 9.042  | 67.578 | -6.278  | 1.00 | 29.82 |
| ATOM | 1794 | C   | GLN A | 225 | 6.105  | 69.126 | -9.858  | 1.00 | 27.45 |
| ATOM | 1795 | O   | GLN A | 225 | 5.503  | 68.056 | -9.759  | 1.00 | 27.59 |
| ATOM | 1796 | N   | SER A | 226 | 6.601  | 69.552 | -11.007 | 1.00 | 27.34 |
| ATOM | 1797 | CA  | SER A | 226 | 6.358  | 68.779 | -12.210 | 1.00 | 28.99 |
| ATOM | 1798 | CB  | SER A | 226 | 5.501  | 69.605 | -13.152 | 1.00 | 28.18 |
| ATOM | 1799 | OG  | SER A | 226 | 5.052  | 68.829 | -14.229 | 1.00 | 40.16 |
| ATOM | 1800 | C   | SER A | 226 | 7.599  | 68.311 | -12.943 | 1.00 | 31.56 |
| ATOM | 1801 | O   | SER A | 226 | 8.570  | 69.055 | -13.087 | 1.00 | 32.05 |
| ATOM | 1802 | N   | ASN A | 227 | 7.571  | 67.055 | -13.370 | 1.00 | 30.89 |
| ATOM | 1803 | CA  | ASN A | 227 | 8.667  | 66.471 | -14.133 | 1.00 | 29.18 |
| ATOM | 1804 | CB  | ASN A | 227 | 8.878  | 67.285 | -15.417 | 1.00 | 28.72 |
| ATOM | 1805 | CG  | ASN A | 227 | 9.511  | 66.482 | -16.528 | 1.00 | 27.74 |
| ATOM | 1806 | OD1 | ASN A | 227 | 9.130  | 65.341 | -16.779 | 1.00 | 28.75 |
| ATOM | 1807 | ND2 | ASN A | 227 | 10.454 | 67.089 | -17.229 | 1.00 | 27.94 |
| ATOM | 1808 | C   | ASN A | 227 | 9.990  | 66.328 | -13.380 | 1.00 | 28.97 |
| ATOM | 1809 | O   | ASN A | 227 | 11.052 | 66.517 | -13.960 | 1.00 | 30.10 |
| ATOM | 1810 | N   | VAL A | 228 | 9.929  | 66.006 | -12.091 | 1.00 | 29.20 |
| ATOM | 1811 | CA  | VAL A | 228 | 11.135 | 65.809 | -11.291 | 1.00 | 27.27 |
| ATOM | 1812 | CB  | VAL A | 228 | 11.599 | 67.058 | -10.497 | 1.00 | 26.29 |
| ATOM | 1813 | CG1 | VAL A | 228 | 13.083 | 67.241 | -10.649 | 1.00 | 23.43 |
| ATOM | 1814 | CG2 | VAL A | 228 | 10.827 | 68.292 | -10.859 | 1.00 | 25.97 |
| ATOM | 1815 | C   | VAL A | 228 | 10.799 | 64.826 | -10.206 | 1.00 | 31.99 |
| ATOM | 1816 | O   | VAL A | 228 | 9.651  | 64.760 | -9.758  | 1.00 | 35.97 |
| ATOM | 1817 | N   | GLN A | 229 | 11.822 | 64.110 | -9.753  | 1.00 | 34.06 |
| ATOM | 1818 | CA  | GLN A | 229 | 11.715 | 63.153 | -8.658  | 1.00 | 33.36 |
| ATOM | 1819 | CB  | GLN A | 229 | 11.795 | 61.734 | -9.176  | 1.00 | 37.53 |
| ATOM | 1820 | CG  | GLN A | 229 | 11.559 | 60.666 | -8.148  | 1.00 | 42.23 |
| ATOM | 1821 | CD  | GLN A | 229 | 11.207 | 59.368 | -8.833  | 1.00 | 55.26 |

|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 1822 | OE1 | GLN A | 229 | 10.110 | 59.222 | -9.392 | 1.00 | 58.46 |
| ATOM | 1823 | NE2 | GLN A | 229 | 12.155 | 58.436 | -8.857 | 1.00 | 59.25 |
| ATOM | 1824 | C   | GLN A | 229 | 12.935 | 63.474 | -7.814 | 1.00 | 34.22 |
| ATOM | 1825 | O   | GLN A | 229 | 14.044 | 63.042 | -8.124 | 1.00 | 34.78 |
| ATOM | 1826 | N   | ASN A | 230 | 12.733 | 64.293 | -6.784 | 1.00 | 34.28 |
| ATOM | 1827 | CA  | ASN A | 230 | 13.827 | 64.732 | -5.917 | 1.00 | 32.42 |
| ATOM | 1828 | C8  | ASN A | 230 | 14.171 | 66.199 | -6.226 | 1.00 | 27.53 |
| ATOM | 1829 | CG  | ASN A | 230 | 12.974 | 67.136 | -6.068 | 1.00 | 21.96 |
| ATOM | 1830 | OD1 | ASN A | 230 | 11.933 | 66.751 | -5.545 | 1.00 | 24.46 |
| ATOM | 1831 | ND2 | ASN A | 230 | 13.118 | 68.361 | -6.541 | 1.00 | 19.87 |
| ATOM | 1832 | C   | ASN A | 230 | 13.575 | 64.587 | -4.419 | 1.00 | 31.95 |
| ATOM | 1833 | O   | ASN A | 230 | 14.476 | 64.808 | -3.622 | 1.00 | 30.47 |
| ATOM | 1834 | N   | LEU A | 231 | 12.356 | 64.231 | -4.034 | 1.00 | 31.28 |
| ATOM | 1835 | CA  | LEU A | 231 | 12.018 | 64.092 | -2.626 | 1.00 | 27.98 |
| ATOM | 1836 | CB  | LEU A | 231 | 10.551 | 64.431 | -2.408 | 1.00 | 24.65 |
| ATOM | 1837 | CG  | LEU A | 231 | 10.254 | 65.884 | -2.135 | 1.00 | 21.29 |
| ATOM | 1838 | CD1 | LEU A | 231 | 8.807  | 65.985 | -1.745 | 1.00 | 24.61 |
| ATOM | 1839 | CD2 | LEU A | 231 | 11.116 | 66.349 | -0.993 | 1.00 | 23.04 |
| ATOM | 1840 | C   | LEU A | 231 | 12.276 | 62.719 | -2.040 | 1.00 | 30.04 |
| ATOM | 1841 | O   | LEU A | 231 | 12.145 | 61.706 | -2.725 | 1.00 | 34.74 |
| ATOM | 1842 | N   | GLN A | 232 | 12.615 | 62.693 | -0.754 | 1.00 | 30.14 |
| ATOM | 1843 | CA  | GLN A | 232 | 12.834 | 61.4iS | -0.034 | 1.00 | 26.30 |
| ATOM | 1844 | CB  | GLN A | 232 | 14.314 | 61.087 | 0.000  | 1.00 | 25.18 |
| ATOM | 1845 | CG  | GLN A | 232 | 14.877 | 60.607 | -1.315 | 1.00 | 24.42 |
| ATOM | 1846 | CD  | GLN A | 232 | 16.251 | 59.976 | -1.163 | 1.00 | 28.50 |
| ATOM | 1847 | OE1 | GLN A | 232 | 17.149 | 60.543 | -0.538 | 1.00 | 29.12 |
| ATOM | 1848 | NE2 | GLN A | 232 | 16.420 | 58.794 | -1.736 | 1.00 | 27.79 |
| ATOM | 1849 | C   | GLN A | 232 | 12.313 | 61.614 | 1.392  | 1.00 | 27.21 |
| ATOM | 1850 | O   | GLN A | 232 | 12.538 | 62.656 | 2.015  | 1.00 | 39.07 |
| ATOM | 1851 | N   | VAL A | 233 | 11.581 | 60.618 | 1.888  | 1.00 | 25.56 |
| ATOM | 1852 | CA  | VAL A | 233 | 11.047 | 60.659 | 3.250  | 1.00 | 23.90 |
| ATOM | 1853 | CB  | VAL A | 233 | 9.588  | 60.195 | 3.354  | 1.00 | 26.06 |
| ATOM | 1854 | CG1 | VAL A | 233 | 8.862  | 61.027 | 4.382  | 1.00 | 28.07 |
| ATOM | 1855 | CG2 | VAL A | 233 | 8.911  | 60.178 | 2.027  | 1.00 | 25.39 |
| ATOM | 1856 | C   | VAL A | 233 | 11.779 | 59.644 | 4.101  | 1.00 | 27.04 |
| ATOM | 1857 | O   | VAL A | 233 | 12.024 | 58.519 | 3.662  | 1.00 | 27.08 |
| ATOM | 1858 | N   | GLU A | 234 | 12.090 | 60.015 | 5.331  | 1.00 | 27.08 |
| ATOM | 1859 | CA  | GLU A | 234 | 12.744 | 59.089 | 6.226  | 1.00 | 28.63 |
| ATOM | 1860 | CB  | GLU A | 234 | 13.512 | 59.848 | 7.289  | 1.00 | 28.65 |
| ATOM | 1861 | CG  | GLU A | 234 | 14.044 | 58.977 | 8.400  | 1.00 | 33.81 |
| ATOM | 1862 | CD  | GLU A | 234 | 14.652 | 59.788 | 9.509  | 1.00 | 37.83 |
| ATOM | 1863 | OE1 | GLU A | 234 | 15.893 | 59.870 | 9.558  | 1.00 | 46.49 |
| ATOM | 1864 | OE2 | GLU A | 234 | 13.894 | 60.356 | 10.323 | 1.00 | 41.82 |
| ATOM | 1865 | C   | GLU A | 234 | 11.637 | 58.292 | 6.881  | 1.00 | 32.99 |
| ATOM | 1866 | O   | GLU A | 234 | 10.761 | 58.861 | 7.526  | 1.00 | 36.86 |
| ATOM | 1867 | N   | THR A | 235 | 11.619 | 56.990 | 6.654  | 1.00 | 39.05 |
| ATOM | 1868 | CA  | THR A | 235 | 10.603 | 56.144 | 7.264  | 1.00 | 43.64 |
| ATOM | 1869 | CB  | THR A | 235 | 9.789  | 55.370 | 6.196  | 1.00 | 47.64 |
| ATOM | 1870 | OG1 | THR A | 235 | 10.663 | 54.518 | 5.443  | 1.00 | 48.96 |
| ATOM | 1871 | CG2 | THR A | 235 | 9.077  | 56.340 | 5.245  | 1.00 | 49.04 |
| ATOM | 1872 | C   | THR A | 235 | 11.310 | 55.161 | 8.186  | 1.00 | 45.27 |
| ATOM | 1873 | O   | THR A | 235 | 12.533 | 55.204 | 8.330  | 1.00 | 46.15 |
| ATOM | 1874 | N   | ALA A | 236 | 10.549 | 54.266 | 8.802  | 1.00 | 48.85 |
| ATOM | 1875 | CA  | ALA A | 236 | 11.131 | 53.271 | 9.697  | 1.00 | 51.37 |
| ATOM | 1876 | CB  | ALA A | 236 | 10.035 | 52.506 | 10.416 | 1.00 | 52.57 |
| ATOM | 1877 | C   | ALA A | 236 | 12.049 | 52.307 | 8.944  | 1.00 | 51.92 |
| ATOM | 1878 | O   | ALA A | 236 | 12.709 | 51.464 | 9.547  | 1.00 | 56.47 |
| ATOM | 1879 | N   | ALA A | 237 | 12.044 | 52.402 | 7.620  | 1.00 | 50.60 |
| ATOM | 1880 | CA  | ALA A | 237 | 12.886 | 51.558 | 6.786  | 1.00 | 50.28 |
| ATOM | 1881 | CB  | ALA A | 237 | 12.044 | 50.870 | 5.720  | 1.00 | 45.48 |
| ATOM | 1882 | C   | ALA A | 237 | 13.952 | 52.421 | 6.126  | 1.00 | 51.53 |
| ATOM | 1883 | O   | ALA A | 237 | 14.591 | 51.992 | 5.156  | 1.00 | 53.02 |
| ATOM | 1884 | N   | GLY A | 238 | 14.159 | 53.620 | 6.672  | 1.00 | 49.22 |
| ATOM | 1885 | CA  | GLY A | 238 | 15.129 | 54.542 | 6.108  | 1.00 | 47.88 |
| ATOM | 1886 | C   | GLY A | 238 | 14.493 | 55.410 | 5.029  | 1.00 | 46.36 |
| ATOM | 1887 | O   | GLY A | 238 | 13.275 | 55.377 | 4.837  | 1.00 | 45.44 |
| ATOM | 1888 | N   | TYR A | 239 | 15.305 | 56.193 | 4.325  | 1.00 | 43.94 |
| ATOM | 1889 | CA  | TYR A | 239 | 14.795 | 57.077 | 3.282  | 1.00 | 42.31 |
| ATOM | 1890 | CB  | TYR A | 239 | 15.860 | 58.079 | 2.862  | 1.00 | 34.38 |
| ATOM | 1891 | CG  | TYR A | 239 | 16.054 | 59.203 | 3.846  | 1.00 | 31.86 |
| ATOM | 1892 | CD1 | TYR A | 239 | 16.902 | 59.064 | 4.943  | 1.00 | 29.03 |
| ATOM | 1893 | CE1 | TYR A | 239 | 17.115 | 60.129 | 5.825  | 1.00 | 30.21 |
| ATOM | 1894 | CD2 | TYR A | 239 | 15.416 | 60.427 | 3.659  | 1.00 | 31.58 |

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|      |      |     |       |     |        |        |         |      |       |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 1895 | CE2 | TYR A | 239 | 15.618 | 61.491 | 4.536   | 1.00 | 27.77 |
| ATOM | 1896 | CZ  | TYR A | 239 | 16.467 | 61.337 | 5.609   | 1.00 | 28.27 |
| ATOM | 1897 | OH  | TYR A | 239 | 16.670 | 62.396 | 6.459   | 1.00 | 30.28 |
| ATOM | 1898 | C   | TYR A | 239 | 14.282 | 56.345 | 2.053   | 1.00 | 44.25 |
| ATOM | 1899 | O   | TYR A | 239 | 14.958 | 55.464 | 1.519   | 1.00 | 50.07 |
| ATOM | 1900 | N   | GLN A | 240 | 13.089 | 56.730 | 1.605   | 1.00 | 42.95 |
| ATOM | 1901 | CA  | GLN A | 240 | 12.457 | 56.135 | 0.434   | 1.00 | 37.56 |
| ATOM | 1902 | CB  | GLN A | 240 | 11.227 | 55.338 | 0.829   | 1.00 | 37.90 |
| ATOM | 1903 | CG  | GLN A | 240 | 11.492 | 54.283 | 1.867   | 1.00 | 39.00 |
| ATOM | 1904 | CD  | GLN A | 240 | 10.259 | 53.503 | 2.178   | 1.00 | 41.54 |
| ATOM | 1905 | OE1 | GLN A | 240 | 9.361  | 53.975 | 2.876   | 1.00 | 42.44 |
| ATOM | 1906 | NE2 | GLN A | 240 | 10.192 | 52.303 | 1.655   | 1.00 | 43.71 |
| ATOM | 1907 | C   | GLN A | 240 | 12.036 | 57.238 | -0.493  | 1.00 | 35.12 |
| ATOM | 1908 | O   | GLN A | 240 | 11.637 | 58.310 | -0.049  | 1.00 | 37.16 |
| ATOM | 1909 | N   | ASP A | 241 | 12.106 | 56.963 | -1.786  | 1.00 | 37.65 |
| ATOM | 1910 | CA  | ASP A | 241 | 11.757 | 57.937 | -2.807  | 1.00 | 33.97 |
| ATOM | 1911 | CB  | ASP A | 241 | 12.294 | 57.477 | -4.157  | 1.00 | 36.71 |
| ATOM | 1912 | CG  | ASP A | 241 | 13.768 | 57.725 | -4.305  | 1.00 | 40.53 |
| ATOM | 1913 | OD1 | ASP A | 241 | 14.501 | 56.767 | -4.626  | 1.00 | 48.07 |
| ATOM | 1914 | OD2 | ASP A | 241 | 14.193 | 58.883 | -4.102  | 1.00 | 43.60 |
| ATOM | 1915 | C   | ASP A | 241 | 10.273 | 58.187 | -2.937  | 1.00 | 31.87 |
| ATOM | 1916 | O   | ASP A | 241 | 9.473  | 57.290 | -2.715  | 1.00 | 33.89 |
| ATOM | 1917 | N   | ILE A | 242 | 9.910  | 59.420 | -3.270  | 1.00 | 29.50 |
| ATOM | 1918 | CA  | ILE A | 242 | 8.516  | 59.776 | -3.491  | 1.00 | 29.59 |
| ATOM | 1919 | CB  | ILE A | 242 | 8.122  | 61.110 | -2.793  | 1.00 | 25.82 |
| ATOM | 1920 | CG2 | ILE A | 242 | 6.718  | 61.540 | -3.205  | 1.00 | 21.57 |
| ATOM | 1921 | CG1 | ILE A | 242 | 8.142  | 60.940 | -1.275  | 1.00 | 22.34 |
| ATOM | 1922 | CD1 | ILE A | 242 | 7.931  | 62.219 | -0.529  | 1.00 | 19.47 |
| ATOM | 1923 | C   | ILE A | 242 | 8.314  | 59.899 | -5.002  | 1.00 | 32.14 |
| ATOM | 1924 | O   | ILE-A | 242 | 9.039  | 60.631 | -5.680  | 1.00 | 34.26 |
| ATOM | 1925 | N   | GLU A | 243 | 7.364  | 59.139 | -5.528  | 1.00 | 32.42 |
| ATOM | 1926 | CA  | GLU A | 243 | 7.051  | 59.161 | -6.950  | 1.00 | 35.87 |
| ATOM | 1927 | CB  | GLU A | 243 | 5.998  | 58.103 | -7.257  | 1.00 | 45.32 |
| ATOM | 1928 | CG  | GLU A | 243 | 4.620  | 58.422 | -6.675  | 1.00 | 58.52 |
| ATOM | 1929 | CD  | GLU A | 243 | 3.584  | 57.359 | -6.970  | 1.00 | 67.74 |
| ATOM | 1930 | OE1 | GLU A | 243 | 2.679  | 57.157 | -6.126  | 1.00 | 72.36 |
| ATOM | 1931 | OE2 | GLU A | 243 | 3.669  | 56.730 | -8.048  | 1.00 | 73.67 |
| ATOM | 1932 | C   | GLU A | 243 | 6.494  | 60.520 | -7.361  | 1.00 | 34.26 |
| ATOM | 1933 | O   | GLU A | 243 | 5.794  | 61.170 | -6.587  | 1.00 | 34.70 |
| ATOM | 1934 | N   | ALA A | 244 | 6.796  | 60.940 | -8.582  | 1.00 | 37.14 |
| ATOM | 1935 | CA  | ALA A | 244 | 6.299  | 62.211 | -9.106  | 1.00 | 36.70 |
| ATOM | 1936 | CB  | ALA A | 244 | 7.187  | 62.704 | -10.237 | 1.00 | 30.95 |
| ATOM | 1937 | C   | ALA A | 244 | 4.870  | 62.045 | -9.607  | 1.00 | 38.29 |
| ATOM | 1938 | O   | ALA A | 244 | 4.401  | 60.919 | -9.809  | 1.00 | 39.49 |
| ATOM | 1939 | N   | ASP A | 245 | 4.184  | 63.168 | -9.810  | 1.00 | 38.94 |
| ATOM | 1940 | CA  | ASP A | 245 | 2.809  | 63.171 | -10.302 | 1.00 | 36.20 |
| ATOM | 1941 | CB  | ASP A | 245 | 1.849  | 62.683 | -9.217  | 1.00 | 35.69 |
| ATOM | 1942 | CG  | ASP A | 245 | 0.436  | 62.479 | -9.730  | 1.00 | 39.12 |
| ATOM | 1943 | OD1 | ASP A | 245 | -0.090 | 63.350 | -10.446 | 1.00 | 38.32 |
| ATOM | 1944 | OD2 | ASP A | 245 | -0.162 | 61.440 | -9.406  | 1.00 | 44.34 |
| ATOM | 1945 | C   | ASP A | 245 | 2.423  | 64.579 | -10.720 | 1.00 | 36.64 |
| ATOM | 1946 | O   | ASP A | 245 | 1.881  | 65.338 | -9.920  | 1.00 | 40.34 |
| ATOM | 1947 | N   | ASP A | 246 | 2.624  | 64.906 | -11.989 | 1.00 | 36.70 |
| ATOM | 1948 | CA  | ASP A | 246 | 2.288  | 66.242 | -12.464 | 1.00 | 42.59 |
| ATOM | 1949 | C8  | ASP A | 246 | 2.956  | 66.546 | -13.815 | 1.00 | 52.74 |
| ATOM | 1950 | CG  | ASP A | 246 | 2.651  | 65.508 | -14.899 | 1.00 | 62.16 |
| ATOM | 1951 | OD1 | ASP A | 246 | 3.484  | 65.398 | -15.834 | 1.00 | 67.79 |
| ATOM | 1952 | OD2 | ASP A | 246 | 1.600  | 64.822 | -14.836 | 1.00 | 61.80 |
| ATOM | 1953 | C   | ASP A | 246 | 0.818  | 66.649 | -12.495 | 1.00 | 39.27 |
| ATOM | 1954 | O   | ASP A | 246 | 0.485  | 67.699 | -13.042 | 1.00 | 39.09 |
| ATOM | 1955 | N   | THR A | 247 | -0.058 | 65.849 | -11.897 | 1.00 | 37.20 |
| ATOM | 1956 | CA  | THR A | 247 | -1.479 | 66.182 | -11.876 | 1.00 | 37.88 |
| ATOM | 1957 | CB  | THR A | 247 | -2.345 | 65.074 | -12.545 | 1.00 | 41.31 |
| ATOM | 1958 | OG1 | THR A | 247 | -2.370 | 63.901 | -11.719 | 1.00 | 44.54 |
| ATOM | 1959 | CG2 | THR A | 247 | -1.770 | 64.688 | -13.903 | 1.00 | 42.77 |
| ATOM | 1960 | C   | THR A | 247 | -1.990 | 66.436 | -10.452 | 1.00 | 37.12 |
| ATOM | 1961 | O   | THR A | 247 | -3.109 | 66.933 | -10.263 | 1.00 | 35.84 |
| ATOM | 1962 | N   | GLY A | 248 | -1.162 | 66.136 | -9.453  | 1.00 | 33.34 |
| ATOM | 1963 | CA  | GLY A | 248 | -1.580 | 66.320 | -8.076  | 1.00 | 29.08 |
| ATOM | 1964 | C   | GLY A | 248 | -0.704 | 67.236 | -7.251  | 1.00 | 26.86 |
| ATOM | 1965 | O   | GLY A | 248 | 0.338  | 67.693 | -7.709  | 1.00 | 29.61 |
| ATOM | 1966 | N   | TYR A | 249 | -1.168 | 67.553 | -6.052  | 1.00 | 24.24 |
| ATOM | 1967 | CA  | TYR A | 249 | -0.432 | 68.401 | -5.128  | 1.00 | 22.26 |

|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 1968 | CB  | TYR A | 249 | -1.319 | 69.512 | -4.571 | 1.00 | 17.04 |
| ATOM | 1969 | CG  | TYR A | 249 | -1.337 | 70.775 | -5.395 | 1.00 | 19.97 |
| ATOM | 1970 | CD1 | TYR A | 249 | -2.159 | 70.896 | -6.505 | 1.00 | 21.32 |
| ATOM | 1971 | CE1 | TYR A | 249 | -2.194 | 72.078 | -7.247 | 1.00 | 22.14 |
| ATOM | 1972 | CD2 | TYR A | 249 | -0.545 | 71.866 | -5.045 | 1.00 | 17.14 |
| ATOM | 1973 | CE2 | TYR A | 249 | -0.575 | 73.041 | -5.777 | 1.00 | 18.05 |
| ATOM | 1974 | CZ  | TYR A | 249 | -1.398 | 73.140 | -6.876 | 1.00 | 18.13 |
| ATOM | 1975 | OH  | TYR A | 249 | -1.412 | 74.302 | -7.612 | 1.00 | 23.74 |
| ATOM | 1976 | C   | TYR A | 249 | 0.037  | 67.520 | -3.982 | 1.00 | 24.44 |
| ATOM | 1977 | O   | TYR A | 249 | -0.766 | 66.920 | -3.363 | 1.00 | 25.35 |
| ATOM | 1978 | N   | LEU A | 250 | 1.344  | 67.505 | -3.745 | 1.00 | 21.09 |
| ATOM | 1979 | CA  | LEU A | 250 | 1.908  | 66.720 | -2.664 | 1.00 | 19.72 |
| ATOM | 1980 | CB  | LEU A | 250 | 3.397  | 66.484 | -2.914 | 1.00 | 11.66 |
| ATOM | 1981 | CG  | LEU A | 250 | 4.092  | 65.533 | -1.946 | 1.00 | 13.51 |
| ATOM | 1982 | CD1 | LEU A | 250 | 3.460  | 64.158 | -1.998 | 1.00 | 9.39  |
| ATOM | 1983 | CD2 | LEU A | 250 | 5.536  | 65.450 | -2.310 | 1.00 | 16.26 |
| ATOM | 1984 | C   | LEU A | 250 | 1.683  | 67.475 | -1.349 | 1.00 | 24.50 |
| ATOM | 1985 | O   | LEU A | 250 | 2.160  | 68.606 | -1.176 | 1.00 | 23.74 |
| ATOM | 1986 | N   | ILE A | 251 | 0.953  | 66.847 | -0.432 | 1.00 | 25.00 |
| ATOM | 1987 | CA  | ILE A | 251 | 0.651  | 67.447 | 0.866  | 1.00 | 23.54 |
| ATOM | 1988 | CB  | ILE A | 251 | -0.876 | 67.411 | 1.138  | 1.00 | 21.54 |
| ATOM | 1989 | CG2 | ILE A | 251 | -1.257 | 68.522 | 2.121  | 1.00 | 20.73 |
| ATOM | 1990 | CG1 | ILE A | 251 | -1.670 | 67.562 | -0.169 | 1.00 | 18.11 |
| ATOM | 1991 | CD1 | ILE A | 251 | -1.594 | 68.929 | -0.792 | 1.00 | 15.82 |
| ATOM | 1992 | C   | ILE A | 251 | 1.376  | 66.775 | 2.071  | 1.00 | 25.96 |
| ATOM | 1993 | O   | ILE A | 251 | 1.478  | 65.545 | 2.148  | 1.00 | 22.81 |
| ATOM | 1994 | N   | ASN A | 252 | 1.919  | 67.590 | 2.979  | 1.00 | 27.93 |
| ATOM | 1995 | CA  | ASN A | 252 | 2.583  | 67.097 | 4.190  | 1.00 | 23.28 |
| ATOM | 1996 | CB  | ASN A | 252 | 4.067  | 66.731 | 3.969  | 1.00 | 19.24 |
| ATOM | 1997 | CG  | ASN A | 252 | 4.949  | 67.922 | 3.669  | 1.00 | 15.95 |
| ATOM | 1998 | OD1 | ASN A | 252 | 5.210  | 68.225 | 2.521  | 1.00 | 27.71 |
| ATOM | 1999 | ND2 | ASN A | 252 | 5.482  | 68.544 | 4.698  | 1.00 | 12.20 |
| ATOM | 2000 | C   | ASN A | 252 | 2.417  | 68.107 | 5.321  | 1.00 | 26.77 |
| ATOM | 2001 | O   | ASN A | 252 | 2.046  | 69.258 | 5.079  | 1.00 | 26.57 |
| ATOM | 2002 | N   | CYS A | 253 | 2.621  | 67.649 | 6.555  | 1.00 | 26.39 |
| ATOM | 2003 | CA  | CYS A | 253 | 2.484  | 68.488 | 7.744  | 1.00 | 23.80 |
| ATOM | 2004 | CB  | CYS A | 253 | 2.069  | 67.638 | 8.950  | 1.00 | 26.15 |
| ATOM | 2005 | SG  | CYS A | 253 | 0.326  | 67.176 | 9.038  | 1.00 | 32.10 |
| ATOM | 2006 | C   | CYS A | 253 | 3.758  | 69.222 | 8.107  | 1.00 | 20.68 |
| ATOM | 2007 | O   | CYS A | 253 | 4.853  | 68.766 | 7.810  | 1.00 | 23.52 |
| ATOM | 2008 | N   | GLY A | 254 | 3.601  | 70.371 | 8.740  | 1.00 | 21.10 |
| ATOM | 2009 | CA  | GLY A | 254 | 4.740  | 71.143 | 9.183  | 1.00 | 21.44 |
| ATOM | 2010 | C   | GLY A | 254 | 4.870  | 70.886 | 10.669 | 1.00 | 19.86 |
| ATOM | 2011 | O   | GLY A | 254 | 4.062  | 70.173 | 11.245 | 1.00 | 17.78 |
| ATOM | 2012 | N   | SER A | 255 | 5.839  | 71.492 | 11.325 | 1.00 | 21.03 |
| ATOM | 2013 | CA  | SER A | 255 | 5.996  | 71.237 | 12.737 | 1.00 | 20.86 |
| ATOM | 2014 | CB  | SER A | 255 | 7.348  | 71.742 | 13.225 | 1.00 | 16.65 |
| ATOM | 2015 | OG  | SER A | 255 | 7.529  | 73.096 | 12.870 | 1.00 | 24.84 |
| ATOM | 2016 | C   | SER A | 255 | 4.862  | 71.800 | 13.592 | 1.00 | 25.80 |
| ATOM | 2017 | O   | SER A | 255 | 4.635  | 71.316 | 14.702 | 1.00 | 32.81 |
| ATOM | 2018 | N   | TYR A | 256 | 4.132  | 72.800 | 13.103 | 1.00 | 23.31 |
| ATOM | 2019 | CA  | TYR A | 256 | 3.048  | 73.337 | 13.916 | 1.00 | 22.05 |
| ATOM | 2020 | CB  | TYR A | 256 | 2.453  | 74.597 | 13.320 | 1.00 | 18.59 |
| ATOM | 2021 | CG  | TYR A | 256 | 1.600  | 75.359 | 14.313 | 1.00 | 18.81 |
| ATOM | 2022 | CD1 | TYR A | 256 | 2.181  | 76.147 | 15.301 | 1.00 | 14.81 |
| ATOM | 2023 | CE1 | TYR A | 256 | 1.399  | 76.878 | 16.198 | 1.00 | 18.34 |
| ATOM | 2024 | CD2 | TYR A | 256 | 0.213  | 75.302 | 14.253 | 1.00 | 22.82 |
| ATOM | 2025 | CE2 | TYR A | 256 | -0.586 | 76.029 | 15.151 | 1.00 | 22.41 |
| ATOM | 2026 | CZ  | TYR A | 256 | 0.015  | 76.812 | 16.122 | 1.00 | 22.48 |
| ATOM | 2027 | OH  | TYR A | 256 | -0.777 | 77.531 | 16.994 | 1.00 | 27.35 |
| ATOM | 2028 | C   | TYR A | 256 | 1.946  | 72.303 | 14.160 | 1.00 | 25.24 |
| ATOM | 2029 | O   | TYR A | 256 | 1.377  | 72.250 | 15.249 | 1.00 | 30.73 |
| ATOM | 2030 | N   | MET A | 257 | 1.645  | 71.490 | 13.152 | 1.00 | 25.21 |
| ATOM | 2031 | CA  | MET A | 257 | 0.633  | 70.443 | 13.281 | 1.00 | 25.59 |
| ATOM | 2032 | CB  | MET A | 257 | 0.422  | 69.749 | 11.930 | 1.00 | 23.11 |
| ATOM | 2033 | CG  | MET A | 257 | -0.631 | 68.646 | 11.889 | 1.00 | 23.77 |
| ATOM | 2034 | SD  | MET A | 257 | -2.303 | 69.226 | 12.196 | 1.00 | 29.13 |
| ATOM | 2035 | CE  | MET A | 257 | -2.926 | 69.464 | 10.571 | 1.00 | 21.14 |
| ATOM | 2036 | C   | MET A | 257 | 1.118  | 69.444 | 14.338 | 1.00 | 29.65 |
| ATOM | 2037 | O   | MET A | 257 | 0.348  | 68.996 | 15.182 | 1.00 | 33.68 |
| ATOM | 2038 | N   | ALA A | 258 | 2.410  | 69.139 | 14.324 | 1.00 | 30.20 |
| ATOM | 2039 | CA  | ALA A | 258 | 2.975  | 68.207 | 15.294 | 1.00 | 29.21 |
| ATOM | 2040 | CB  | ALA A | 258 | 4.437  | 67.918 | 14.962 | 1.00 | 26.53 |

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|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 2041 | C   | ALA A | 258 | 2.843  | 68.740 | 16.721 | 1.00 | 29.82 |
| ATOM | 2042 | O   | ALA A | 258 | 2.486  | 67.999 | 17.635 | 1.00 | 30.07 |
| ATOM | 2043 | N   | HIS A | 259 | 3.130  | 70.023 | 16.912 | 1.00 | 29.81 |
| ATOM | 2044 | CA  | HIS A | 259 | 3.023  | 70.635 | 18.231 | 1.00 | 30.03 |
| ATOM | 2045 | CB  | HIS A | 259 | 3.560  | 72.061 | 18.197 | 1.00 | 29.44 |
| ATOM | 2046 | CG  | HIS A | 259 | 3.279  | 72.846 | 19.441 | 1.00 | 36.67 |
| ATOM | 2047 | CD2 | HIS A | 259 | 3.973  | 72.971 | 20.600 | 1.00 | 35.37 |
| ATOM | 2048 | ND1 | HIS A | 259 | 2.174  | 73.662 | 19.572 | 1.00 | 39.99 |
| ATOM | 2049 | CE1 | HIS A | 259 | 2.201  | 74.255 | 20.750 | 1.00 | 40.19 |
| ATOM | 2050 | NE2 | HIS A | 259 | 3.284  | 73.854 | 21.397 | 1.00 | 33.91 |
| ATOM | 2051 | C   | HIS A | 259 | 1.571  | 70.645 | 18.703 | 1.00 | 32.65 |
| ATOM | 2052 | O   | HIS A | 259 | 1.295  | 70.499 | 19.884 | 1.00 | 37.28 |
| ATOM | 2053 | N   | LEU A | 260 | 0.650  | 70.862 | 17.778 | 1.00 | 33.08 |
| ATOM | 2054 | CA  | LEU A | 260 | -0.770 | 70.900 | 18.092 | 1.00 | 31.90 |
| ATOM | 2055 | CB  | LEU A | 260 | -1.543 | 71.402 | 16.880 | 1.00 | 30.79 |
| ATOM | 2056 | CG  | LEU A | 260 | -2.224 | 72.751 | 16.957 | 1.00 | 33.95 |
| ATOM | 2057 | CD1 | LEU A | 260 | -1.342 | 73.763 | 17.664 | 1.00 | 35.15 |
| ATOM | 2058 | CD2 | LEU A | 260 | -2.549 | 73.184 | 15.536 | 1.00 | 39.19 |
| ATOM | 2059 | C   | LEU A | 260 | -1.326 | 69.536 | 18.470 | 1.00 | 33.38 |
| ATOM | 2060 | O   | LEU A | 260 | -2.082 | 69.411 | 19.420 | 1.00 | 35.86 |
| ATOM | 2061 | N   | THR A | 261 | -0.988 | 68.526 | 17.684 | 1.00 | 32.53 |
| ATOM | 2062 | CA  | THR A | 261 | -1.480 | 67.184 | 17.905 | 1.00 | 33.81 |
| ATOM | 2063 | CB  | THR A | 261 | -1.571 | 66.443 | 16.580 | 1.00 | 35.83 |
| ATOM | 2064 | OG1 | THR A | 261 | -0.270 | 66.392 | 15.977 | 1.00 | 33.48 |
| ATOM | 2065 | CG2 | THR A | 261 | -2.537 | 67.155 | 15.647 | 1.00 | 37.64 |
| ATOM | 2066 | C   | THR A | 261 | -0.590 | 66.389 | 18.840 | 1.00 | 39.46 |
| ATOM | 2067 | O   | THR A | 261 | -0.651 | 65.153 | 18.870 | 1.00 | 38.94 |
| ATOM | 2068 | N   | ASN A | 262 | 0.267  | 67.094 | 19.572 | 1.00 | 44.19 |
| ATOM | 2069 | CA  | ASN A | 262 | 1.191  | 66.456 | 20.506 | 1.00 | 49.58 |
| ATOM | 2070 | CB  | ASN A | 262 | 0.445  | 65.952 | 21.756 | 1.00 | 59.13 |
| ATOM | 2071 | CG  | ASN A | 262 | 1.353  | 65.841 | 22.981 | 1.00 | 66.86 |
| ATOM | 2072 | OD1 | ASN A | 262 | 1.367  | 66.737 | 23.833 | 1.00 | 72.04 |
| ATOM | 2073 | ND2 | ASN A | 262 | 2.105  | 64.743 | 23.081 | 1.00 | 67.84 |
| ATOM | 2074 | C   | ASN A | 262 | 1.941  | 65.307 | 19.811 | 1.00 | 46.90 |
| ATOM | 2075 | O   | ASN A | 262 | 2.228  | 64.274 | 20.415 | 1.00 | 49.43 |
| ATOM | 2076 | N   | ASN A | 263 | 2.208  | 65.492 | 18.522 | 1.00 | 41.44 |
| ATOM | 2077 | CA  | ASN A | 263 | 2.929  | 64.534 | 17.698 | 1.00 | 37.52 |
| ATOM | 2078 | C13 | ASN A | 263 | 4.237  | 64.119 | 18.347 | 1.00 | 41.11 |
| ATOM | 2079 | CG  | ASN A | 263 | 5.415  | 64.740 | 17.670 | 1.00 | 47.69 |
| ATOM | 2080 | OD1 | ASN A | 263 | 5.928  | 65.764 | 18.109 | 1.00 | 48.68 |
| ATOM | 2081 | ND2 | ASN A | 263 | 5.824  | 64.155 | 16.550 | 1.00 | 54.33 |
| ATOM | 2082 | C   | ASN A | 263 | 2.201  | 63.322 | 17.172 | 1.00 | 35.18 |
| ATOM | 2083 | O   | ASN A | 263 | 2.832  | 62.388 | 16.679 | 1.00 | 34.27 |
| ATOM | 2084 | N   | TYR A | 264 | 0.877  | 63.344 | 17.250 | 1.00 | 36.95 |
| ATOM | 2085 | CA  | TYR A | 264 | 0.063  | 62.252 | 16.723 | 1.00 | 37.39 |
| ATOM | 2086 | CB  | TYR A | 264 | -1.393 | 62.413 | 17.189 | 1.00 | 33.82 |
| ATOM | 2087 | CG  | TYR A | 264 | -2.344 | 61.342 | 16.713 | 1.00 | 33.63 |
| ATOM | 2088 | CD1 | TYR A | 264 | -2.446 | 60.113 | 17.362 | 1.00 | 32.49 |
| ATOM | 2089 | CE1 | TYR A | 264 | -3.375 | 59.551 | 16.935 | 1.00 | 33.06 |
| ATOM | 2090 | CD2 | TYR A | 264 | -3.180 | 61.579 | 15.627 | 1.00 | 37.61 |
| ATOM | 2091 | CE2 | TYR A | 264 | -4.105 | 60.636 | 15.195 | 1.00 | 37.45 |
| ATOM | 2092 | CZ  | TYR A | 264 | -4.204 | 59.429 | 15.845 | 1.00 | 35.62 |
| ATOM | 2093 | OH  | TYR A | 264 | -5.169 | 58.546 | 15.403 | 1.00 | 38.87 |
| ATOM | 2094 | C   | TYR A | 264 | 0.218  | 62.311 | 15.186 | 1.00 | 37.01 |
| ATOM | 2095 | O   | TYR A | 264 | 0.169  | 61.287 | 14.499 | 1.00 | 37.37 |
| ATOM | 2096 | N   | TYR A | 265 | 0.390  | 63.528 | 14.666 | 1.00 | 36.23 |
| ATOM | 2097 | CA  | TYR A | 265 | 0.642  | 63.768 | 13.244 | 1.00 | 33.20 |
| ATOM | 2098 | CB  | TYR A | 265 | -0.351 | 64.750 | 12.640 | 1.00 | 26.57 |
| ATOM | 2099 | CG  | TYR A | 265 | -1.642 | 64.115 | 12.239 | 1.00 | 31.72 |
| ATOM | 2100 | CD1 | TYR A | 265 | -2.630 | 64.861 | 11.610 | 1.00 | 33.04 |
| ATOM | 2101 | CE1 | TYR A | 265 | -3.854 | 64.298 | 11.286 | 1.00 | 30.94 |
| ATOM | 2102 | CD2 | TYR A | 265 | -1.909 | 62.775 | 12.527 | 1.00 | 32.98 |
| ATOM | 2103 | CE2 | TYR A | 265 | -3.141 | 62.201 | 12.207 | 1.00 | 31.76 |
| ATOM | 2104 | CZ  | TYR A | 265 | -4.102 | 62.976 | 11.591 | 1.00 | 30.37 |
| ATOM | 2105 | OH  | TYR A | 265 | -5.333 | 62.452 | 11.312 | 1.00 | 38.15 |
| ATOM | 2106 | C   | TYR A | 265 | 2.028  | 64.390 | 13.227 | 1.00 | 34.58 |
| ATOM | 2107 | O   | TYR A | 265 | 2.187  | 65.586 | 13.466 | 1.00 | 35.29 |
| ATOM | 2108 | N   | LYS A | 266 | 3.036  | 63.553 | 13.022 | 1.00 | 34.31 |
| ATOM | 2109 | CA  | LYS A | 266 | 4.422  | 63.990 | 13.002 | 1.00 | 33.62 |
| ATOM | 2110 | CB  | LYS A | 266 | 5.328  | 62.772 | 13.039 | 1.00 | 39.20 |
| ATOM | 2111 | CG  | LYS A | 266 | 6.739  | 63.066 | 13.491 | 1.00 | 56.22 |
| ATOM | 2112 | CD  | LYS A | 266 | 7.549  | 61.773 | 13.584 | 1.00 | 67.11 |
| ATOM | 2113 | CE  | LYS A | 266 | 6.797  | 60.697 | 14.372 | 1.00 | 74.71 |

|      |      |     |       |     |        |        |         |      |       |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 2114 | NZ  | LYS A | 266 | 6.402  | 61.147 | 15.748  | 1.00 | 80.37 |
| ATOM | 2115 | C   | LYS A | 266 | 4.748  | 64.784 | 11.759  | 1.00 | 29.29 |
| ATOM | 2116 | O   | LYS A | 266 | 4.184  | 64.540 | 10.702  | 1.00 | 30.14 |
| ATOM | 2117 | N   | ALA A | 267 | 5.641  | 65.752 | 11.890  | 1.00 | 26.90 |
| ATOM | 2118 | CA  | ALA A | 267 | 6.063  | 66.526 | 10.735  | 1.00 | 27.00 |
| ATOM | 2119 | CB  | ALA A | 267 | 6.724  | 67.809 | 11.173  | 1.00 | 22.67 |
| ATOM | 2120 | C   | ALA A | 267 | 7.079  | 65.599 | 10.072  | 1.00 | 28.13 |
| ATOM | 2121 | O   | ALA A | 267 | 8.074  | 65.243 | 10.695  | 1.00 | 31.38 |
| ATOM | 2122 | N   | PRO A | 268 | 6.822  | 65.155 | 8.823   | 1.00 | 30.02 |
| ATOM | 2123 | CD  | PRO A | 268 | 5.648  | 65.466 | 7.989   | 1.00 | 29.53 |
| ATOM | 2124 | Q   | PRO A | 268 | 7.732  | 64.251 | 8.103   | 1.00 | 28.12 |
| ATOM | 2125 | CB  | PRO A | 268 | 7.043  | 64.081 | 6.742   | 1.00 | 25.57 |
| ATOM | 2126 | CG  | PRO A | 268 | 5.615  | 64.286 | 7.035   | 1.00 | 25.50 |
| ATOM | 2127 | C   | PRO A | 268 | 9.133  | 64.805 | 7.904   | 1.00 | 27.55 |
| ATOM | 2128 | O   | PRO A | 268 | 9.281  | 65.974 | 7.555   | 1.00 | 31.71 |
| ATOM | 2129 | N   | ILE A | 269 | 10.153 | 63.984 | 8.156   | 1.00 | 26.79 |
| ATOM | 2130 | Q   | ILE A | 269 | 11.549 | 64.374 | 7.939   | 1.00 | 21.70 |
| ATOM | 2131 | CB  | ILE A | 269 | 12.527 | 63.535 | 8.799   | 1.00 | 23.68 |
| ATOM | 2132 | CG2 | ILE A | 269 | 13.971 | 63.768 | 8.358   | 1.00 | 16.90 |
| ATOM | 2133 | CG1 | ILE A | 269 | 12.371 | 63.881 | 10.286  | 1.00 | 25.36 |
| ATOM | 2134 | CD1 | ILE A | 269 | 12.761 | 65.311 | 10.645  | 1.00 | 21.95 |
| ATOM | 2135 | C   | ILE A | 269 | 11.788 | 64.052 | 6.470   | 1.00 | 21.77 |
| ATOM | 2136 | O   | ILE A | 269 | 11.544 | 62.932 | 6.025   | 1.00 | 23.31 |
| ATOM | 2137 | N   | HIS A | 270 | 12.196 | 65.043 | 5.696   | 1.00 | 22.73 |
| ATOM | 2138 | CA  | HIS A | 270 | 12.420 | 64.808 | 4.280   | 1.00 | 21.55 |
| ATOM | 2139 | CB  | HIS A | 270 | 11.161 | 65.146 | 3.480   | 1.00 | 20.47 |
| ATOM | 2140 | CG  | HIS A | 270 | 10.613 | 66.507 | 3.758   | 1.00 | 16.63 |
| ATOM | 2141 | CD2 | HIS A | 270 | 10.417 | 67.570 | 2.946   | 1.00 | 20.91 |
| ATOM | 2142 | ND1 | HIS A | 270 | 10.148 | 66.885 | 4.997   | 1.00 | 18.74 |
| ATOM | 2143 | CE1 | HIS A | 270 | 9.680  | 68.117 | 4.936   | 1.00 | 20.88 |
| ATOM | 2144 | NE2 | HIS A | 270 | 9.828  | 68.559 | 3.700   | 1.00 | 17.58 |
| ATOM | 2145 | C   | HIS A | 270 | 13.608 | 65.600 | 3.783   | 1.00 | 22.67 |
| ATOM | 2146 | O   | HIS A | 270 | 14.008 | 66.588 | 4.410   | 1.00 | 23.83 |
| ATOM | 2147 | N   | ARG A | 271 | 14.201 | 65.136 | 2.689   | 1.00 | 20.85 |
| ATOM | 2148 | CA  | ARG A | 271 | 15.359 | 65.797 | 2.093   | 1.00 | 23.79 |
| ATOM | 2149 | CB  | ARG A | 271 | 16.631 | 65.043 | 2.461   | 1.00 | 22.83 |
| ATOM | 2150 | CG  | ARG A | 271 | 16.615 | 63.592 | 2.057   | 1.00 | 23.45 |
| ATOM | 2151 | CD  | ARG A | 271 | 17.872 | 62.894 | 2.523   | 1.00 | 25.22 |
| ATOM | 2152 | NE  | ARG A | 271 | 18.020 | 61.603 | 1.862   | 1.00 | 26.89 |
| ATOM | 2153 | CZ  | ARG A | 271 | 19.008 | 60.753 | 2.103   | 1.00 | 25.53 |
| ATOM | 2154 | NH1 | ARG A | 271 | 19.931 | 61.058 | 2.996   | 1.00 | 29.48 |
| ATOM | 2155 | NH2 | ARG A | 271 | 19.081 | 59.607 | 1.441   | 1.00 | 25.73 |
| ATOM | 2156 | C   | ARG A | 271 | 15.190 | 65.873 | 0.580   | 1.00 | 23.68 |
| ATOM | 2157 | O   | ARG A | 271 | 14.319 | 65.211 | 0.010   | 1.00 | 26.81 |
| ATOM | 2158 | N   | VAL A | 272 | 15.994 | 66.702 | -0.071  | 1.00 | 22.19 |
| ATOM | 2159 | Q   | VAL A | 272 | 15.878 | 66.857 | -1.510  | 1.00 | 18.76 |
| ATOM | 2160 | CB  | VAL A | 272 | 15.561 | 68.310 | -1.870  | 1.00 | 17.63 |
| ATOM | 2161 | CG1 | VAL A | 272 | 15.326 | 68.446 | -3.355  | 1.00 | 18.50 |
| ATOM | 2162 | CG2 | VAL A | 272 | 14.340 | 68.778 | -1.107  | 1.00 | 15.11 |
| ATOM | 2163 | C   | VAL A | 272 | 17.132 | 66.418 | -2.248  | 1.00 | 25.28 |
| ATOM | 2164 | O   | VAL A | 272 | 18.202 | 66.993 | -2.050  | 1.00 | 29.40 |
| ATOM | 2165 | N   | LYS A | 273 | 16.985 | 65.396 | -3.092  | 1.00 | 27.72 |
| ATOM | 2166 | CA  | LYS A | 273 | 18.059 | 64.845 | -3.919  | 1.00 | 25.89 |
| ATOM | 2167 | CB  | LYS A | 273 | 17.572 | 63.587 | -4.645  | 1.00 | 27.95 |
| ATOM | 2168 | CG  | LYS A | 273 | 17.355 | 62.392 | -3.753  | 1.00 | 31.66 |
| ATOM | 2169 | CD  | LYS A | 273 | 16.404 | 61.385 | -4.376  | 1.00 | 35.66 |
| ATOM | 2170 | CE  | LYS A | 273 | 16.963 | 60.740 | -5.621  | 1.00 | 41.21 |
| ATOM | 2171 | NZ  | LYS A | 273 | 16.185 | 59.514 | -5.974  | 1.00 | 42.41 |
| ATOM | 2172 | C   | LYS A | 273 | 18.551 | 65.837 | -4.968  | 1.00 | 25.96 |
| ATOM | 2173 | O   | LYS A | 273 | 17.784 | 66.653 | -5.486  | 1.00 | 26.05 |
| ATOM | 2174 | N   | TRP A | 274 | 19.843 | 65.759 | -5.268  | 1.00 | 25.99 |
| ATOM | 2175 | Q   | TRP A | 274 | 20.4S9 | 66.616 | -6.267  | 1.00 | 24.01 |
| ATOM | 2176 | CB  | TRP A | 274 | 21.975 | 66.623 | -6.096  | 1.00 | 24.20 |
| ATOM | 2177 | CG  | TRP A | 274 | 22.700 | 67.347 | -7.187  | 1.00 | 23.66 |
| ATOM | 2178 | CD2 | TRP A | 274 | 23.526 | 66.762 | -8.194  | 1.00 | 21.71 |
| ATOM | 2179 | CE2 | TRP A | 274 | 23.997 | 67.812 | -9.008  | 1.00 | 21.28 |
| ATOM | 2180 | CE3 | TRP A | 274 | 23.900 | 65.453 | -8.498  | 1.00 | 25.08 |
| ATOM | 2181 | CD1 | TRP A | 274 | 22.709 | 68.689 | -7.417  | 1.00 | 26.21 |
| ATOM | 2182 | NE1 | TRP A | 274 | 23.490 | 68.979 | -8.509  | 1.00 | 28.27 |
| ATOM | 2183 | CZ2 | TRP A | 274 | 24.839 | 67.594 | -10.089 | 1.00 | 23.56 |
| ATOM | 2184 | CZ3 | TRP A | 274 | 24.739 | 65.237 | -9.582  | 1.00 | 29.23 |
| ATOM | 2185 | CH2 | TRP A | 274 | 25.193 | 66.305 | -10.367 | 1.00 | 24.09 |
| ATOM | 2186 | C   | TRP A | 274 | 20.105 | 66.099 | -7.653  | 1.00 | 27.26 |

|      |      |     |       |     |        |        |         |      |       |
|------|------|-----|-------|-----|--------|--------|---------|------|-------|
| ATOM | 2187 | O   | TRP A | 274 | 20.357 | 64.938 | -7.970  | 1.00 | 32.63 |
| ATOM | 2188 | N   | VAL A | 275 | 19.503 | 66.964 | -8.461  | 1.00 | 28.27 |
| ATOM | 2189 | CA  | VAL A | 275 | 19.110 | 66.636 | -9.825  | 1.00 | 25.56 |
| ATOM | 2190 | CB  | VAL A | 275 | 17.582 | 66.606 | -9.971  | 1.00 | 23.27 |
| ATOM | 2191 | CG1 | VAL A | 275 | 17.200 | 66.358 | -11.410 | 1.00 | 23.05 |
| ATOM | 2192 | CG2 | VAL A | 275 | 16.993 | 65.545 | -9.073  | 1.00 | 25.58 |
| ATOM | 2193 | C   | VAL A | 275 | 19.645 | 67.760 | -10.689 | 1.00 | 23.04 |
| ATOM | 2194 | O   | VAL A | 275 | 19.194 | 68.884 | -10.573 | 1.00 | 27.65 |
| ATOM | 2195 | N   | ASN A | 276 | 20.627 | 67.480 | -11.532 | 1.00 | 24.79 |
| ATOM | 2196 | CA  | ASN A | 276 | 21.172 | 68.539 | -12.372 | 1.00 | 23.43 |
| ATOM | 2197 | CB  | ASN A | 276 | 22.626 | 68.262 | -12.737 | 1.00 | 23.64 |
| ATOM | 2198 | CG  | ASN A | 276 | 23.237 | 69.374 | -13.563 | 1.00 | 27.31 |
| ATOM | 2199 | OD1 | ASN A | 276 | 22.697 | 70.479 | -13.650 | 1.00 | 25.48 |
| ATOM | 2200 | ND2 | ASN A | 276 | 24.382 | 69.096 | -14.156 | 1.00 | 32.14 |
| ATOM | 2201 | C   | ASN A | 276 | 20.347 | 68.732 | -13.632 | 1.00 | 24.63 |
| ATOM | 2202 | O   | ASN A | 276 | 20.683 | 68.215 | -14.694 | 1.00 | 31.02 |
| ATOM | 2203 | N   | ALA A | 277 | 19.244 | 69.453 | -13.499 | 1.00 | 25.78 |
| ATOM | 2204 | CA  | ALA A | 277 | 18.364 | 69.719 | -14.620 | 1.00 | 23.03 |
| ATOM | 2205 | CB  | ALA A | 277 | 17.502 | 68.507 | -14.911 | 1.00 | 26.09 |
| ATOM | 2206 | C   | ALA A | 277 | 17.490 | 70.903 | -14.288 | 1.00 | 25.78 |
| ATOM | 2207 | O   | ALA A | 277 | 17.232 | 71.177 | -13.119 | 1.00 | 27.01 |
| ATOM | 2208 | N   | GLU A | 278 | 17.034 | 71.602 | -15.321 | 1.00 | 25.92 |
| ATOM | 2209 | CA  | GLU A | 278 | 16.176 | 72.760 | -15.139 | 1.00 | 27.97 |
| ATOM | 2210 | CB  | GLU A | 278 | 16.111 | 73.616 | -16.399 | 1.00 | 29.38 |
| ATOM | 2211 | CG  | GLU A | 278 | 17.326 | 74.473 | -16.634 | 1.00 | 34.40 |
| ATOM | 2212 | CD  | GLU A | 278 | 17.373 | 75.697 | -15.764 | 1.00 | 31.39 |
| ATOM | 2213 | OE1 | GLU A | 278 | 16.312 | 76.182 | -15.327 | 1.00 | 35.93 |
| ATOM | 2214 | OE2 | GLU A | 278 | 18.489 | 76.186 | -15.537 | 1.00 | 37.93 |
| ATOM | 2215 | C   | GLU A | 278 | 14.777 | 72.323 | -14.767 | 1.00 | 30.01 |
| ATOM | 2216 | O   | GLU A | 278 | 13.999 | 71.867 | -15.601 | 1.00 | 33.28 |
| ATOM | 2217 | N   | ARG A | 279 | 14.485 | 72.419 | -13.487 | 1.00 | 30.78 |
| ATOM | 2218 | CA  | ARG A | 279 | 13.185 | 72.069 | -12.986 | 1.00 | 29.39 |
| ATOM | 2219 | CB  | ARG A | 279 | 13.232 | 70.718 | -12.294 | 1.00 | 29.88 |
| ATOM | 2220 | CG  | ARG A | 279 | 13.756 | 69.606 | -13.168 | 1.00 | 29.15 |
| ATOM | 2221 | CD  | ARG A | 279 | 12.891 | 69.382 | -14.381 | 1.00 | 26.70 |
| ATOM | 2222 | NE  | ARG A | 279 | 13.340 | 68.183 | -15.073 | 1.00 | 28.42 |
| ATOM | 2223 | CZ  | ARG A | 279 | 13.978 | 68.185 | -16.234 | 1.00 | 25.05 |
| ATOM | 2224 | NH1 | ARG A | 279 | 14.224 | 69.324 | -16.855 | 1.00 | 21.11 |
| ATOM | 2225 | NH2 | ARG A | 279 | 14.477 | 67.059 | -16.716 | 1.00 | 26.84 |
| ATOM | 2226 | C   | ARG A | 279 | 12.813 | 73.163 | -12.007 | 1.00 | 30.45 |
| ATOM | 2227 | O   | ARG A | 279 | 13.645 | 74.001 | -11.643 | 1.00 | 28.64 |
| ATOM | 2228 | N   | GLN A | 280 | 11.560 | 73.147 | -11.583 | 1.00 | 31.12 |
| ATOM | 2229 | CA  | GLN A | 280 | 11.045 | 74.134 | -10.661 | 1.00 | 33.15 |
| ATOM | 2230 | CB  | GLN A | 280 | 10.260 | 75.182 | -11.427 | 1.00 | 38.18 |
| ATOM | 2231 | CG  | GLN A | 280 | 9.171  | 74.580 | -12.286 | 1.00 | 53.46 |
| ATOM | 2232 | CD  | GLN A | 280 | 8.596  | 75.565 | -13.278 | 1.00 | 57.41 |
| ATOM | 2233 | OE1 | GLN A | 280 | 9.209  | 76.593 | -13.568 | 1.00 | 60.52 |
| ATOM | 2234 | NE2 | GLN A | 280 | 7.418  | 75.250 | -13.820 | 1.00 | 60.10 |
| ATOM | 2235 | C   | GLN A | 280 | 10.138 | 73.430 | -9.679  | 1.00 | 30.33 |
| ATOM | 2236 | O   | GLN A | 280 | 9.602  | 72.363 | -9.975  | 1.00 | 32.02 |
| ATOM | 2237 | N   | SER A | 281 | 9.958  | 74.049 | -8.521  | 1.00 | 26.28 |
| ATOM | 2238 | CA  | SER A | 281 | 9.131  | 73.510 | -7.462  | 1.00 | 18.83 |
| ATOM | 2239 | CB  | SER A | 281 | 10.034 | 72.908 | -6.390  | 1.00 | 16.21 |
| ATOM | 2240 | OG  | SER A | 281 | 9.281  | 72.175 | -5.458  | 1.00 | 31.28 |
| ATOM | 2241 | C   | SER A | 281 | 8.344  | 74.691 | -6.918  | 1.00 | 17.91 |
| ATOM | 2242 | O   | SER A | 281 | 8.870  | 75.796 | -6.852  | 1.00 | 15.21 |
| ATOM | 2243 | N   | LEU A | 282 | 7.070  | 74.487 | -6.596  | 1.00 | 24.14 |
| ATOM | 2244 | CA  | LEU A | 282 | 6.239  | 75.578 | -6.068  | 1.00 | 24.06 |
| ATOM | 2245 | CB  | LEU A | 282 | 5.224  | 76.049 | -7.098  | 1.00 | 26.03 |
| ATOM | 2246 | CG  | LEU A | 282 | 5.733  | 76.662 | -8.388  | 1.00 | 34.69 |
| ATOM | 2247 | CD1 | LEU A | 282 | 6.212  | 75.564 | -9.339  | 1.00 | 37.28 |
| ATOM | 2248 | CD2 | LEU A | 282 | 4.582  | 77.421 | -9.009  | 1.00 | 38.00 |
| ATOM | 2249 | C   | LEU A | 282 | 5.480  | 75.182 | -4.814  | 1.00 | 23.88 |
| ATOM | 2250 | O   | LEU A | 282 | 4.368  | 74.652 | -4.894  | 1.00 | 21.16 |
| ATOM | 2251 | N   | PRO A | 283 | 6.109  | 75.372 | -3.637  | 1.00 | 22.81 |
| ATOM | 2252 | CD  | PRO A | 283 | 7.531  | 75.682 | -3.434  | 1.00 | 22.38 |
| ATOM | 2253 | CA  | PRO A | 283 | 5.463  | 75.035 | -2.372  | 1.00 | 20.82 |
| ATOM | 2254 | CB  | PRO A | 283 | 6.661  | 74.739 | -1.472  | 1.00 | 18.71 |
| ATOM | 2255 | CG  | PRO A | 283 | 7.663  | 75.746 | -1.928  | 1.00 | 19.17 |
| ATOM | 2256 | C   | PRO A | 283 | 4.651  | 76.192 | -1.847  | 1.00 | 17.56 |
| ATOM | 2257 | O   | PRO A | 283 | 5.028  | 77.349 | -2.001  | 1.00 | 19.99 |
| ATOM | 2258 | N   | PHE A | 284 | 3.496  | 75.874 | -1.282  | 1.00 | 18.04 |
| ATOM | 2259 | CA  | PHE A | 284 | 2.628  | 76.869 | -0.686  | 1.00 | 14.83 |

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|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 2260 | CB  | PHE A | 284 | 1.202  | 76.739 | -1.221 | 1.00 | 13.11 |
| ATOM | 2261 | CG  | PHE A | 284 | 0.222  | 77.695 | -0.590 | 1.00 | 9.51  |
| ATOM | 2262 | CD1 | PHE A | 284 | 0.361  | 79.072 | -0.757 | 1.00 | 7.91  |
| ATOM | 2263 | CD2 | PHE A | 284 | -0.840 | 77.218 | 0.176  | 1.00 | 8.25  |
| ATOM | 2264 | CE1 | PHE A | 284 | -0.546 | 79.963 | -0.172 | 1.00 | 9.04  |
| ATOM | 2265 | CE2 | PHE A | 284 | -1.755 | 78.103 | 0.769  | 1.00 | 7.90  |
| ATOM | 2266 | CZ  | PHE A | 284 | -1.607 | 79.480 | 0.596  | 1.00 | 7.48  |
| ATOM | 2267 | C   | PHE A | 284 | 2.657  | 76.481 | 0.777  | 1.00 | 15.38 |
| ATOM | 2268 | O   | PHE A | 284 | 2.315  | 75.351 | 1.126  | 1.00 | 13.28 |
| ATOM | 2269 | N   | PHE A | 285 | 3.130  | 77.381 | 1.625  | 1.00 | 11.26 |
| ATOM | 2270 | CA  | PHE A | 285 | 3.204  | 77.096 | 3.045  | 1.00 | 11.08 |
| ATOM | 2271 | CB  | PHE A | 285 | 4.488  | 77.682 | 3.622  | 1.00 | 11.89 |
| ATOM | 2272 | CG  | PHE A | 285 | 5.734  | 77.103 | 3.021  | 1.00 | 13.37 |
| ATOM | 2273 | CD1 | PHE A | 285 | 6.418  | 77.779 | 2.024  | 1.00 | 12.80 |
| ATOM | 2274 | CD2 | PHE A | 285 | 6.229  | 75.882 | 3.458  | 1.00 | 14.08 |
| ATOM | 2275 | CE1 | PHE A | 285 | 7.584  | 77.245 | 1.477  | 1.00 | 16.30 |
| ATOM | 2276 | CE2 | PHE A | 285 | 7.396  | 75.347 | 2.911  | 1.00 | 13.47 |
| ATOM | 2277 | CZ  | PHE A | 285 | 8.066  | 76.030 | 1.925  | 1.00 | 7.59  |
| ATOM | 2278 | C   | PHE A | 285 | 1.985  | 77.644 | 3.756  | 1.00 | 12.95 |
| ATOM | 2279 | O   | PHE A | 285 | 1.781  | 78.863 | 3.801  | 1.00 | 14.08 |
| ATOM | 2280 | N   | VAL A | 286 | 1.150  | 76.746 | 4.271  | 1.00 | 11.34 |
| ATOM | 2281 | CA  | VAL A | 286 | -0.062 | 77.158 | 4.969  | 1.00 | 15.20 |
| ATOM | 2282 | CB  | VAL A | 286 | -1.128 | 76.021 | 4.997  | 1.00 | 13.61 |
| ATOM | 2283 | CG1 | VAL A | 286 | -2.365 | 76.467 | 5.739  | 1.00 | 11.57 |
| ATOM | 2284 | CG2 | VAL A | 286 | -1.511 | 75.629 | 3.587  | 1.00 | 10.57 |
| ATOM | 2285 | C   | VAL A | 286 | 0.271  | 77.647 | 6.384  | 1.00 | 18.76 |
| ATOM | 2286 | O   | VAL A | 286 | 0.667  | 76.876 | 7.257  | 1.00 | 24.10 |
| ATOM | 2287 | N   | ASN A | 287 | 0.190  | 78.955 | 6.571  | 1.00 | 17.87 |
| ATOM | 2288 | CA  | ASN A | 287 | 0.461  | 79.568 | 7.850  | 1.00 | 18.13 |
| ATOM | 2289 | CB  | ASN A | 287 | 1.570  | 80.621 | 7.722  | 1.00 | 19.63 |
| ATOM | 2290 | CG  | ASN A | 287 | 2.940  | 80.017 | 7.427  | 1.00 | 17.67 |
| ATOM | 2291 | OD1 | ASN A | 287 | 3.287  | 78.940 | 7.907  | 1.00 | 15.97 |
| ATOM | 2292 | ND2 | ASN A | 287 | 3.729  | 80.727 | 6.644  | 1.00 | 19.12 |
| ATOM | 2293 | C   | ASN A | 287 | -0.844 | 80.242 | 8.229  | 1.00 | 21.86 |
| ATOM | 2294 | O   | ASN A | 287 | -1.584 | 80.680 | 7.347  | 1.00 | 26.85 |
| ATOM | 2295 | N   | LEU A | 288 | -1.148 | 80.302 | 9.523  | 1.00 | 19.51 |
| ATOM | 2296 | CA  | LEU A | 288 | -2.374 | 80.928 | 9.979  | 1.00 | 14.83 |
| ATOM | 2297 | CB  | LEU A | 288 | -2.853 | 80.254 | 11.253 | 1.00 | 12.62 |
| ATOM | 2298 | CG  | LEU A | 288 | -2.982 | 78.741 | 11.075 | 1.00 | 17.68 |
| ATOM | 2299 | CD1 | LEU A | 288 | -3.540 | 78.114 | 12.332 | 1.00 | 16.20 |
| ATOM | 2300 | CD2 | LEU A | 288 | -3.883 | 78.428 | 9.909  | 1.00 | 14.63 |
| ATOM | 2301 | C   | LEU A | 288 | -2.139 | 82.414 | 10.188 | 1.00 | 16.91 |
| ATOM | 2302 | O   | LEU A | 288 | -1.218 | 82.981 | 9.611  | 1.00 | 20.51 |
| ATOM | 2303 | N   | GLY A | 289 | -2.974 | 83.051 | 10.996 | 1.00 | 16.67 |
| ATOM | 2304 | CA  | GLY A | 289 | -2.823 | 84.473 | 11.240 | 1.00 | 15.37 |
| ATOM | 2305 | C   | GLY A | 289 | -1.831 | 84.700 | 12.350 | 1.00 | 19.82 |
| ATOM | 2306 | O   | GLY A | 289 | -1.571 | 83.795 | 13.130 | 1.00 | 22.79 |
| ATOM | 2307 | N   | TYR A | 290 | -1.342 | 85.924 | 12.477 | 1.00 | 19.69 |
| ATOM | 2308 | CA  | TYR A | 290 | -0.354 | 86.246 | 13.491 | 1.00 | 23.55 |
| ATOM | 2309 | CB  | TYR A | 290 | 0.058  | 87.705 | 13.359 | 1.00 | 22.89 |
| ATOM | 2310 | CG  | TYR A | 290 | 1.265  | 88.073 | 14.184 | 1.00 | 30.95 |
| ATOM | 2311 | CD1 | TYR A | 290 | 2.558  | 87.793 | 13.730 | 1.00 | 31.65 |
| ATOM | 2312 | CE1 | TYR A | 290 | 3.671  | 88.142 | 14.481 | 1.00 | 32.74 |
| ATOM | 2313 | CD2 | TYR A | 290 | 1.122  | 88.710 | 15.414 | 1.00 | 29.60 |
| ATOM | 2314 | CE2 | TYR A | 290 | 2.228  | 89.063 | 16.172 | 1.00 | 31.69 |
| ATOM | 2315 | CZ  | TYR A | 290 | 3.494  | 88.778 | 15.699 | 1.00 | 32.60 |
| ATOM | 2316 | OH  | TYR A | 290 | 4.587  | 89.149 | 16.435 | 1.00 | 38.35 |
| ATOM | 2317 | C   | TYR A | 290 | -0.825 | 85.973 | 14.912 | 1.00 | 28.88 |
| ATOM | 2318 | O   | TYR A | 290 | -0.064 | 85.469 | 15.747 | 1.00 | 32.22 |
| ATOM | 2319 | N   | ASP A | 291 | -2.080 | 86.302 | 15.180 | 1.00 | 32.16 |
| ATOM | 2320 | CA  | ASP A | 291 | -2.650 | 86.121 | 16.505 | 1.00 | 34.89 |
| ATOM | 2321 | CB  | ASP A | 291 | -3.621 | 87.271 | 16.809 | 1.00 | 44.67 |
| ATOM | 2322 | CG  | ASP A | 291 | -2.907 | 88.607 | 17.064 | 1.00 | 54.47 |
| ATOM | 2323 | OD1 | ASP A | 291 | -1.678 | 88.612 | 17.294 | 1.00 | 62.50 |
| ATOM | 2324 | OD2 | ASP A | 291 | -3.583 | 89.662 | 17.057 | 1.00 | 59.68 |
| ATOM | 2325 | C   | ASP A | 291 | -3.341 | 84.786 | 16.743 | 1.00 | 33.13 |
| ATOM | 2326 | O   | ASP A | 291 | -3.867 | 84.552 | 17.828 | 1.00 | 36.71 |
| ATOM | 2327 | N   | SER A | 292 | -3.325 | 83.902 | 15.755 | 1.00 | 32.93 |
| ATOM | 2328 | CA  | SER A | 292 | -3.989 | 82.611 | 15.896 | 1.00 | 33.04 |
| ATOM | 2329 | CB  | SER A | 292 | -4.074 | 81.892 | 14.551 | 1.00 | 32.62 |
| ATOM | 2330 | OG  | SER A | 292 | -4.870 | 82.629 | 13.641 | 1.00 | 37.64 |
| ATOM | 2331 | C   | SER A | 292 | -3.394 | 81.675 | 16.933 | 1.00 | 33.50 |
| ATOM | 2332 | O   | SER A | 292 | -2.223 | 81.310 | 16.870 | 1.00 | 35.88 |

|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 2333 | N   | VAL A | 293 | -4.323 | 81.283 | 17.889 | 1.00 | 35.69 |
| ATOM | 2334 | CA  | VAL A | 293 | -3.807 | 80.371 | 18.936 | 1.00 | 33.43 |
| ATOM | 2335 | CB  | VAL A | 293 | -3.867 | 81.015 | 20.333 | 1.00 | 28.87 |
| ATOM | 2336 | CG1 | VAL A | 293 | -3.244 | 80.086 | 21.346 | 1.00 | 29.10 |
| ATOM | 2337 | CG2 | VAL A | 293 | -3.157 | 82.350 | 20.340 | 1.00 | 28.79 |
| ATOM | 2338 | C   | VAL A | 293 | -4.754 | 79.193 | 18.925 | 1.00 | 33.08 |
| ATOM | 2339 | O   | VAL A | 293 | -5.971 | 79.366 | 18.990 | 1.00 | 33.77 |
| ATOM | 2340 | N   | ILE A | 294 | -4.187 | 78.002 | 18.790 | 1.00 | 34.36 |
| ATOM | 2341 | CA  | ILE A | 294 | -4.952 | 76.770 | 18.784 | 1.00 | 33.14 |
| ATOM | 2342 | CB  | ILE A | 294 | -4.754 | 76.000 | 17.458 | 1.00 | 33.14 |
| ATOM | 2343 | CG2 | ILE A | 294 | -5.426 | 74.629 | 17.518 | 1.00 | 28.09 |
| ATOM | 2344 | CG1 | ILE A | 294 | -5.318 | 76.832 | 16.303 | 1.00 | 29.00 |
| ATOM | 2345 | CD1 | ILE A | 294 | -5.328 | 76.129 | 14.973 | 1.00 | 30.92 |
| ATOM | 2346 | C   | ILE A | 294 | -4.476 | 75.952 | 19.983 | 1.00 | 36.82 |
| ATOM | 2347 | O   | ILE A | 294 | -3.277 | 75.882 | 20.273 | 1.00 | 40.13 |
| ATOM | 2348 | N   | ASP A | 295 | -5.427 | 75.385 | 20.710 | 1.00 | 37.77 |
| ATOM | 2349 | CA  | ASP A | 295 | -5.124 | 74.604 | 21.889 | 1.00 | 36.56 |
| ATOM | 2350 | CB  | ASP A | 295 | -6.346 | 74.499 | 22.783 | 1.00 | 42.24 |
| ATOM | 2351 | CG  | ASP A | 295 | -6.163 | 75.234 | 24.071 | 1.00 | 50.87 |
| ATOM | 2352 | OD1 | ASP A | 295 | -6.049 | 74.565 | 25.117 | 1.00 | 60.02 |
| ATOM | 2353 | OD2 | ASP A | 295 | -6.092 | 76.481 | 24.038 | 1.00 | 55.86 |
| ATOM | 2354 | C   | ASP A | 295 | -4.655 | 73.223 | 21.544 | 1.00 | 35.69 |
| ATOM | 2355 | O   | ASP A | 295 | -5.384 | 72.453 | 20.928 | 1.00 | 35.08 |
| ATOM | 2356 | N   | PRO A | 296 | -3.431 | 72.879 | 21.955 | 1.00 | 35.13 |
| ATOM | 2357 | CD  | PRO A | 296 | -2.488 | 73.736 | 22.692 | 1.00 | 34.11 |
| ATOM | 2358 | CA  | PRO A | 296 | -2.847 | 71.563 | 21.690 | 1.00 | 35.32 |
| ATOM | 2359 | CB  | PRO A | 296 | -1.478 | 71.653 | 22.368 | 1.00 | 33.77 |
| ATOM | 2360 | CG  | PRO A | 296 | -1.169 | 73.116 | 22.339 | 1.00 | 35.72 |
| ATOM | 2361 | C   | PRO A | 296 | -3.689 | 70.463 | 22.327 | 1.00 | 38.35 |
| ATOM | 2362 | O   | PRO A | 296 | -4.269 | 70.653 | 23.394 | 1.00 | 38.55 |
| ATOM | 2363 | N   | PHE A | 297 | -3.706 | 69.300 | 21.697 | 1.00 | 37.27 |
| ATOM | 2364 | CA  | PHE A | 297 | -4.455 | 68.180 | 22.208 | 1.00 | 34.45 |
| ATOM | 2365 | CB  | PHE A | 297 | -5.877 | 68.209 | 21.654 | 1.00 | 31.82 |
| ATOM | 2366 | CG  | PHE A | 297 | -5.957 | 68.187 | 20.151 | 1.00 | 30.97 |
| ATOM | 2367 | CD1 | PHE A | 297 | -6.324 | 67.025 | 19.475 | 1.00 | 31.48 |
| ATOM | 2368 | CD2 | PHE A | 297 | -5.712 | 69.339 | 19.414 | 1.00 | 30.11 |
| ATOM | 2369 | CE1 | PHE A | 297 | -6.445 | 67.018 | 18.083 | 1.00 | 29.97 |
| ATOM | 2370 | CE2 | PHE A | 297 | -5.832 | 69.338 | 18.023 | 1.00 | 30.13 |
| ATOM | 2371 | CZ  | PHE A | 297 | -6.200 | 68.177 | 17.358 | 1.00 | 40.88 |
| ATOM | 2372 | C   | PHE A | 297 | -3.770 | 66.887 | 21.809 | 1.00 | 43.86 |
| ATOM | 2373 | O   | PHE A | 297 | -2.954 | 66.865 | 20.891 | 1.00 | 44.53 |
| ATOM | 2374 | N   | ASP A | 298 | -4.064 | 65.806 | 22.511 | 1.00 | 48.48 |
| ATOM | 2375 | CA  | ASP A | 298 | -3.466 | 64.534 | 22.167 | 1.00 | 52.93 |
| ATOM | 2376 | CB  | ASP A | 298 | -2.590 | 64.015 | 23.295 | 1.00 | 57.44 |
| ATOM | 2377 | CG  | ASP A | 298 | -1.808 | 62.778 | 22.898 | 1.00 | 54.35 |
| ATOM | 2378 | OD1 | ASP A | 298 | -2.020 | 62.254 | 21.778 | 1.00 | 66.50 |
| ATOM | 2379 | OD2 | ASP A | 298 | -0.964 | 62.333 | 23.705 | 1.00 | 50.22 |
| ATOM | 2380 | C   | ASP A | 298 | -4.584 | 63.552 | 21.907 | 1.00 | 49.77 |
| ATOM | 2381 | O   | ASP A | 298 | -5.215 | 63.067 | 22.827 | 1.00 | 52.46 |
| ATOM | 2382 | N   | PRO A | 299 | -4.789 | 63.199 | 20.630 | 1.00 | 52.72 |
| ATOM | 2383 | CD  | PRO A | 299 | -4.105 | 63.730 | 19.439 | 1.00 | 56.64 |
| ATOM | 2384 | CA  | PRO A | 299 | -5.835 | 62.266 | 20.230 | 1.00 | 54.35 |
| ATOM | 2385 | CB  | PRO A | 299 | -5.663 | 62.206 | 18.717 | 1.00 | 50.07 |
| ATOM | 2386 | CG  | PRO A | 299 | -5.165 | 63.564 | 18.388 | 1.00 | 63.86 |
| ATOM | 2387 | C   | PRO A | 299 | -5.648 | 60.898 | 20.868 | 1.00 | 69.53 |
| ATOM | 2388 | O   | PRO A | 299 | -6.492 | 60.011 | 20.687 | 1.00 | 68.69 |
| ATOM | 2389 | N   | MG A  | 300 | -4.535 | 60.712 | 21.580 | 1.00 | 73.13 |
| ATOM | 2390 | CA  | ARG A | 300 | -4.231 | 59.449 | 22.250 | 1.00 | 73.05 |
| ATOM | 2391 | CB  | ARG A | 300 | -2.731 | 59.153 | 22.191 | 1.00 | 75.18 |
| ATOM | 2392 | CG  | ARG A | 300 | -2.202 | 58.825 | 20.810 | 1.00 | 72.55 |
| ATOM | 2393 | CD  | ARG A | 300 | -0.682 | 58.842 | 20.790 | 1.00 | 71.35 |
| ATOM | 2394 | NE  | ARG A | 300 | -0.165 | 60.144 | 21.181 | 1.00 | 71.94 |
| ATOM | 2395 | CZ  | ARG A | 300 | 0.867  | 60.748 | 20.595 | 1.00 | 73.46 |
| ATOM | 2396 | NH1 | ARG A | 300 | 1.506  | 60.171 | 19.579 | 1.00 | 71.10 |
| ATOM | 2397 | NH2 | ARG A | 300 | 1.274  | 61.934 | 21.032 | 1.00 | 76.43 |
| ATOM | 2398 | C   | ARG A | 300 | -4.685 | 59.414 | 23.708 | 1.00 | 80.12 |
| ATOM | 2399 | O   | ARG A | 300 | -4.552 | 58.390 | 24.374 | 1.00 | 77.10 |
| ATOM | 2400 | N   | GLU A | 301 | -5.202 | 60.536 | 24.196 | 1.00 | 81.37 |
| ATOM | 2401 | CA  | GLU A | 301 | -5.687 | 60.596 | 25.562 | 1.00 | 82.38 |
| ATOM | 2402 | CB  | GLU A | 301 | -4.984 | 61.711 | 26.331 | 1.00 | 89.06 |
| ATOM | 2403 | CG  | GLU A | 301 | -3.474 | 61.523 | 26.422 | 1.00 | 94.30 |
| ATOM | 2404 | CD  | GLU A | 301 | -2.918 | 62.004 | 27.750 | 1.00 | 97.83 |
| ATOM | 2405 | OE1 | GLU A | 301 | -3.152 | 63.179 | 28.115 | 1.00 |       |

|      |      |     |       |     |         |        |        |      |       |
|------|------|-----|-------|-----|---------|--------|--------|------|-------|
| ATOM | 2406 | OE2 | GLU A | 301 | -2.241  | 61.201 | 28.425 | 1.00 | 97.36 |
| ATOM | 2407 | C   | GLU A | 301 | -7.193  | 60.781 | 25.642 | 1.00 | 84.64 |
| ATOM | 2408 | O   | GLU A | 301 | -7.779  | 61.498 | 24.836 | 1.00 | 83.56 |
| ATOM | 2409 | N   | PRO A | 302 | -7.849  | 60.122 | 26.611 | 1.00 | 88.29 |
| ATOM | 2410 | CD  | PRO A | 302 | -7.263  | 59.114 | 27.527 | 1.00 | 89.03 |
| ATOM | 2411 | CA  | PRO A | 302 | -9.303  | 60.201 | 26.800 | 1.00 | 87.98 |
| ATOM | 2412 | CB  | PRO A | 302 | -9.521  | 59.416 | 28.095 | 1.00 | 88.81 |
| ATOM | 2413 | CG  | PRO A | 302 | -8.478  | 58.337 | 27.978 | 1.00 | 88.81 |
| ATOM | 2414 | C   | PRO A | 302 | -9.804  | 61.652 | 26.925 | 1.00 | 86.15 |
| ATOM | 2415 | O   | PRO A | 302 | -10.737 | 62.060 | 26.236 | 1.00 | 85.57 |
| ATOM | 2416 | N   | ASN A | 303 | -9.184  | 62.425 | 27.817 | 1.00 | 84.86 |
| ATOM | 2417 | CA  | ASN A | 303 | -9.563  | 63.822 | 27.985 | 1.00 | 85.24 |
| ATOM | 2418 | CB  | ASN A | 303 | -8.929  | 64.404 | 29.254 | 1.00 | 89.02 |
| ATOM | 2419 | CG  | ASN A | 303 | -9.217  | 65.900 | 29.433 | 1.00 | 93.08 |
| ATOM | 2420 | OD1 | ASN A | 303 | -8.501  | 66.589 | 30.150 | 1.00 | 95.61 |
| ATOM | 2421 | ND2 | ASN A | 303 | -10.242 | 66.401 | 28.755 | 1.00 | 95.94 |
| ATOM | 2422 | C   | ASN A | 303 | -9.073  | 64.602 | 26.773 | 1.00 | 83.46 |
| ATOM | 2423 | O   | ASN A | 303 | -9.678  | 65.601 | 26.377 | 1.00 | 82.51 |
| ATOM | 2424 | N   | GLY A | 304 | -8.001  | 64.099 | 26.169 | 1.00 | 82.29 |
| ATOM | 2425 | CA  | GLY A | 304 | -7.413  | 64.745 | 25.016 | 1.00 | 79.23 |
| ATOM | 2426 | C   | GLY A | 304 | -6.639  | 65.945 | 25.513 | 1.00 | 77.89 |
| ATOM | 2427 | O   | GLY A | 304 | -6.503  | 66.945 | 24.802 | 1.00 | 78.97 |
| ATOM | 2428 | N   | LYS A | 305 | -6.156  | 65.855 | 26.748 | 1.00 | 76.87 |
| ATOM | 2429 | CA  | LYS A | 305 | -5.403  | 66.938 | 27.348 | 1.00 | 76.76 |
| ATOM | 2430 | CB  | LYS A | 305 | -5.585  | 66.962 | 28.880 | 1.00 | 78.46 |
| ATOM | 2431 | CG  | LYS A | 305 | -4.408  | 66.440 | 29.691 | 1.00 | 82.23 |
| ATOM | 2432 | CD  | LYS A | 305 | -3.751  | 67.539 | 30.519 | 1.00 | 85.07 |
| ATOM | 2433 | CE  | LYS A | 305 | -2.573  | 66.997 | 31.311 | 1.00 | 88.93 |
| ATOM | 2434 | NZ  | LYS A | 305 | -2.157  | 67.917 | 32.403 | 1.00 | 93.14 |
| ATOM | 2435 | C   | LYS A | 305 | -3.949  | 66.755 | 26.972 | 1.00 | 73.92 |
| ATOM | 2436 | O   | LYS A | 305 | -3.474  | 65.623 | 26.867 | 1.00 | 73.27 |
| ATOM | 2437 | N   | SER A | 306 | -3.237  | 67.855 | 26.797 | 1.00 | 72.39 |
| ATOM | 2438 | CA  | SER A | 306 | -1.844  | 67.787 | 26.417 | 1.00 | 73.15 |
| ATOM | 2439 | CB  | SER A | 306 | -1.656  | 68.461 | 25.061 | 1.00 | 72.57 |
| ATOM | 2440 | OG  | SER A | 306 | -2.237  | 69.762 | 25.069 | 1.00 | 70.16 |
| ATOM | 2441 | C   | SER A | 306 | -0.982  | 68.474 | 27.445 | 1.00 | 73.60 |
| ATOM | 2442 | O   | SER A | 306 | -1.481  | 69.180 | 28.328 | 1.00 | 71.26 |
| ATOM | 2443 | N   | ASP A | 307 | 0.314   | 68.208 | 27.363 | 1.00 | 76.59 |
| ATOM | 2444 | CA  | ASP A | 307 | 1.281   | 68.827 | 28.260 | 1.00 | 78.33 |
| ATOM | 2445 | CB  | ASP A | 307 | 2.480   | 67.891 | 28.515 | 1.00 | 84.92 |
| ATOM | 2446 | CG  | ASP A | 307 | 3.022   | 67.239 | 27.236 | 1.00 | 89.57 |
| ATOM | 2447 | OD1 | ASP A | 307 | 3.809   | 67.902 | 26.515 | 1.00 | 90.72 |
| ATOM | 2448 | OD2 | ASP A | 307 | 2.672   | 66.065 | 26.956 | 1.00 | 74.93 |
| ATOM | 2449 | C   | ASP A | 307 | 1.734   | 70.130 | 27.593 | 1.00 | 73.18 |
| ATOM | 2450 | O   | ASP A | 307 | 1.883   | 71.163 | 28.254 | 1.00 | 70.05 |
| ATOM | 2451 | N   | ARG A | 308 | 1.893   | 70.072 | 26.268 | 1.00 | 64.62 |
| ATOM | 2452 | CA  | ARG A | 308 | 2.327   | 71.212 | 25.471 | 1.00 | 64.91 |
| ATOM | 2453 | CB  | ARG A | 308 | 2.295   | 70.877 | 23.986 | 1.00 | 65.23 |
| ATOM | 2454 | CG  | ARG A | 308 | 3.177   | 69.738 | 23.570 | 1.00 | 65.31 |
| ATOM | 2455 | CD  | ARG A | 308 | 3.284   | 69.720 | 22.067 | 1.00 | 68.52 |
| ATOM | 2456 | NE  | ARG A | 308 | 3.889   | 68.494 | 21.573 | 1.00 | 69.44 |
| ATOM | 2457 | CZ  | ARG A | 308 | 5.145   | 68.139 | 21.800 | 1.00 | 70.73 |
| ATOM | 2458 | NH1 | ARG A | 308 | 5.939   | 68.925 | 22.515 | 1.00 | 71.60 |
| ATOM | 2459 | NH2 | ARG A | 308 | 5.596   | 66.983 | 21.334 | 1.00 | 60.56 |
| ATOM | 2460 | C   | ARG A | 308 | 1.422   | 72.394 | 25.695 | 1.00 | 62.91 |
| ATOM | 2461 | O   | ARG A | 308 | 0.211   | 72.243 | 25.786 | 1.00 | 58.75 |
| ATOM | 2462 | N   | GLU A | 309 | 2.016   | 73.576 | 25.721 | 1.00 | 59.53 |
| ATOM | 2463 | CA  | GLU A | 309 | 1.278   | 74.807 | 25.937 | 1.00 | 64.51 |
| ATOM | 2464 | CB  | GLU A | 309 | 2.155   | 75.795 | 26.707 | 1.00 | 72.73 |
| ATOM | 2465 | CG  | GLU A | 309 | 2.863   | 75.195 | 27.909 | 1.00 | 78.39 |
| ATOM | 2466 | CD  | GLU A | 309 | 4.037   | 76.041 | 28.375 | 1.00 | 80.45 |
| ATOM | 2467 | OE1 | GLU A | 309 | 5.196   | 75.650 | 28.107 | 1.00 | 81.42 |
| ATOM | 2468 | OE2 | GLU A | 309 | 3.802   | 77.091 | 29.013 | 1.00 | 58.18 |
| ATOM | 2469 | C   | GLU A | 309 | 0.895   | 75.423 | 24.595 | 1.00 | 56.69 |
| ATOM | 2470 | O   | GLU A | 309 | 1.550   | 75.172 | 23.576 | 1.00 | 57.07 |
| ATOM | 2471 | N   | PRO A | 310 | -0.202  | 76.204 | 24.566 | 1.00 | 58.98 |
| ATOM | 2472 | CD  | PRO A | 310 | -1.130  | 76.528 | 25.662 | 1.00 | 54.68 |
| ATOM | 2473 | CA  | PRO A | 310 | -0.639  | 76.848 | 23.325 | 1.00 | 56.45 |
| ATOM | 2474 | CB  | PRO A | 310 | -1.898  | 77.610 | 23.755 | 1.00 | 57.32 |
| ATOM | 2475 | CG  | PRO A | 310 | -1.671  | 77.867 | 25.214 | 1.00 | 49.05 |
| ATOM | 2476 | C   | PRO A | 310 | 0.456   | 77.787 | 22.831 | 1.00 | 48.09 |
| ATOM | 2477 | O   | PRO A | 310 | 1.136   | 78.437 | 23.631 | 1.00 | 43.40 |
| ATOM | 2478 | N   | LEU A | 311 | 0.617   | 77.835 | 21.512 | 1.00 |       |

|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 2479 | CA  | LEU A | 311 | 1.626  | 78.650 | 20.859 | 1.00 | 36.12 |
| ATOM | 2480 | CB  | LEU A | 311 | 2.661  | 77.726 | 20.204 | 1.00 | 32.22 |
| ATOM | 2481 | CG  | LEU A | 311 | 3.919  | 78.324 | 19.578 | 1.00 | 31.79 |
| ATOM | 2482 | CD1 | LEU A | 311 | 4.582  | 79.300 | 20.539 | 1.00 | 28.33 |
| ATOM | 2483 | CD2 | LEU A | 311 | 4.862  | 77.194 | 19.229 | 1.00 | 26.30 |
| ATOM | 2484 | C   | LEU A | 311 | 0.936  | 79.478 | 19.793 | 1.00 | 32.51 |
| ATOM | 2485 | O   | LEU A | 311 | 0.300  | 78.915 | 18.903 | 1.00 | 35.00 |
| ATOM | 2486 | N   | SER A | 312 | 1.012  | 80.804 | 19.899 | 1.00 | 27.12 |
| ATOM | 2487 | CA  | SER A | 312 | 0.386  | 81.654 | 18.894 | 1.00 | 26.22 |
| ATOM | 2488 | CB  | SER A | 312 | 0.324  | 83.123 | 19.339 | 1.00 | 22.14 |
| ATOM | 2489 | OG  | SER A | 312 | 1.479  | 83.859 | 19.000 | 1.00 | 31.44 |
| ATOM | 2490 | C   | SER A | 312 | 1.205  | 81.464 | 17.621 | 1.00 | 30.09 |
| ATOM | 2491 | O   | SER A | 312 | 2.438  | 81.349 | 17.671 | 1.00 | 34.62 |
| ATOM | 2492 | N   | TYR A | 313 | 0.526  | 81.399 | 16.483 | 1.00 | 30.05 |
| ATOM | 2493 | CA  | TYR A | 313 | 1.208  | 81.164 | 15.222 | 1.00 | 26.78 |
| ATOM | 2494 | CB  | TYR A | 313 | 0.221  | 81.101 | 14.070 | 1.00 | 21.90 |
| ATOM | 2495 | CG  | TYR A | 313 | 0.740  | 80.223 | 12.968 | 1.00 | 23.94 |
| ATOM | 2496 | CD1 | TYR A | 313 | 0.464  | 78.868 | 12.972 | 1.00 | 20.72 |
| ATOM | 2497 | CE1 | TYR A | 313 | 0.991  | 78.032 | 12.022 | 1.00 | 22.06 |
| ATOM | 2498 | CD2 | TYR A | 313 | 1.555  | 80.729 | 11.951 | 1.00 | 16.61 |
| ATOM | 2499 | CE2 | TYR A | 313 | 2.091  | 79.891 | 10.996 | 1.00 | 16.69 |
| ATOM | 2500 | CZ  | TYR A | 313 | 1.792  | 78.541 | 11.041 | 1.00 | 17.14 |
| ATOM | 2501 | OH  | TYR A | 313 | 2.294  | 77.666 | 10.123 | 1.00 | 24.17 |
| ATOM | 2502 | C   | TYR A | 313 | 2.299  | 82.153 | 14.895 | 1.00 | 25.77 |
| ATOM | 2503 | O   | TYR A | 313 | 3.326  | 81.778 | 14.334 | 1.00 | 23.63 |
| ATOM | 2504 | N   | GLY A | 314 | 2.071  | 83.415 | 15.238 | 1.00 | 28.58 |
| ATOM | 2505 | CA  | GLY A | 314 | 3.053  | 84.444 | 14.965 | 1.00 | 34.94 |
| ATOM | 2506 | C   | GLY A | 314 | 4.370  | 84.186 | 15.674 | 1.00 | 37.23 |
| ATOM | 2507 | O   | GLY A | 314 | 5.434  | 84.453 | 15.117 | 1.00 | 41.94 |
| ATOM | 2508 | N   | ASP A | 315 | 4.301  | 83.683 | 16.906 | 1.00 | 37.16 |
| ATOM | 2509 | CA  | ASP A | 315 | 5.498  | 83.388 | 17.682 | 1.00 | 33.44 |
| ATOM | 2510 | CB  | ASP A | 315 | 5.162  | 83.140 | 19.157 | 1.00 | 37.41 |
| ATOM | 2511 | CG  | ASP A | 315 | 4.707  | 84.406 | 19.881 | 1.00 | 40.95 |
| ATOM | 2512 | OD1 | ASP A | 315 | 3.906  | 84.295 | 20.835 | 1.00 | 48.93 |
| ATOM | 2513 | OD2 | ASP A | 315 | 5.147  | 85.515 | 19.504 | 1.00 | 45.51 |
| ATOM | 2514 | C   | ASP A | 315 | 6.147  | 82.172 | 17.074 | 1.00 | 28.81 |
| ATOM | 2515 | O   | ASP A | 315 | 7.357  | 82.139 | 16.893 | 1.00 | 32.18 |
| ATOM | 2516 | N   | TYR A | 316 | 5.333  | 81.179 | 16.746 | 1.00 | 26.31 |
| ATOM | 2517 | CA  | TYR A | 316 | 5.823  | 79.963 | 16.116 | 1.00 | 25.28 |
| ATOM | 2518 | CB  | TYR A | 316 | 4.646  | 79.064 | 15.709 | 1.00 | 23.80 |
| ATOM | 2519 | CG  | TYR A | 316 | 4.986  | 77.997 | 14.682 | 1.00 | 28.01 |
| ATOM | 2520 | CD1 | TYR A | 316 | 5.604  | 76.802 | 15.061 | 1.00 | 26.83 |
| ATOM | 2521 | CE1 | TYR A | 316 | 5.903  | 75.810 | 14.106 | 1.00 | 25.18 |
| ATOM | 2522 | CD2 | TYR A | 316 | 4.682  | 78.177 | 13.323 | 1.00 | 22.23 |
| ATOM | 2523 | CE2 | TYR A | 316 | 4.981  | 77.194 | 12.372 | 1.00 | 16.07 |
| ATOM | 2524 | CZ  | TYR A | 316 | 5.586  | 76.020 | 12.769 | 1.00 | 19.33 |
| ATOM | 2525 | O8  | TYR A | 316 | 5.850  | 75.040 | 11.843 | 1.00 | 22.12 |
| ATOM | 2526 | C   | TYR A | 316 | 6.625  | 80.333 | 14.872 | 1.00 | 26.20 |
| ATOM | 2527 | O   | TYR A | 316 | 7.812  | 80.010 | 14.766 | 1.00 | 23.86 |
| ATOM | 2528 | N   | LEU A | 317 | 5.977  | 81.062 | 13.966 | 1.00 | 26.87 |
| ATOM | 2529 | CA  | LEU A | 317 | 6.579  | 81.454 | 12.705 | 1.00 | 26.33 |
| ATOM | 2530 | CB  | LEU A | 317 | 5.548  | 82.112 | 11.783 | 1.00 | 22.99 |
| ATOM | 2531 | CG  | LEU A | 317 | 6.032  | 82.167 | 10.334 | 1.00 | 17.66 |
| ATOM | 2532 | CD1 | LEU A | 317 | 5.962  | 80.780 | 9.722  | 1.00 | 16.43 |
| ATOM | 2533 | CD2 | LEU A | 317 | 5.205  | 83.147 | 9.549  | 1.00 | 13.47 |
| ATOM | 2534 | C   | LEU A | 317 | 7.801  | 82.340 | 12.830 | 1.00 | 25.42 |
| ATOM | 2535 | O   | LEU A | 317 | 8.781  | 82.125 | 12.134 | 1.00 | 29.40 |
| ATOM | 2536 | N   | GLN A | 318 | 7.753  | 83.341 | 13.696 | 1.00 | 26.38 |
| ATOM | 2537 | CA  | GLN A | 318 | 8.891  | 84.226 | 13.846 | 1.00 | 29.10 |
| ATOM | 2538 | CB  | GLN A | 318 | 8.643  | 85.254 | 14.933 | 1.00 | 34.57 |
| ATOM | 2539 | CG  | GLN A | 318 | 7.722  | 86.361 | 14.557 | 1.00 | 45.89 |
| ATOM | 2540 | CD  | GLN A | 318 | 7.422  | 87.230 | 15.744 | 1.00 | 54.11 |
| ATOM | 2541 | OE1 | GLN A | 318 | 8.276  | 87.996 | 16.198 | 1.00 | 60.92 |
| ATOM | 2542 | NE2 | GLN A | 318 | 6.224  | 87.084 | 16.292 | 1.00 | 56.69 |
| ATOM | 2543 | C   | GLN A | 318 | 10.114 | 83.429 | 14.215 | 1.00 | 32.19 |
| ATOM | 2544 | O   | GLN A | 318 | 11.147 | 83.529 | 13.560 | 1.00 | 34.97 |
| ATOM | 2545 | N   | ASN A | 319 | 9.967  | 82.589 | 15.231 | 1.00 | 33.42 |
| ATOM | 2546 | CA  | ASN A | 319 | 11.076 | 81.780 | 15.711 | 1.00 | 38.92 |
| ATOM | 2547 | CB  | ASN A | 319 | 10.751 | 81.192 | 17.088 | 1.00 | 45.44 |
| ATOM | 2548 | CG  | ASN A | 319 | 10.635 | 82.276 | 18.174 | 1.00 | 54.83 |
| ATOM | 2549 | OD1 | ASN A | 319 | 11.612 | 82.952 | 18.502 | 1.00 | 56.44 |
| ATOM | 2550 | ND2 | ASN A | 319 | 9.429  | 82.470 | 18.702 | 1.00 | 59.48 |
| ATOM | 2551 | C   | ASN A | 319 | 11.506 | 80.705 | 14.725 | 1.00 | 40.03 |

|      |      |     |       |     |         |        |         |      |       |
|------|------|-----|-------|-----|---------|--------|---------|------|-------|
| ATOM | 2552 | O   | ASN A | 319 | 12.703  | 80.502 | 14.494  | 1.00 | 44.50 |
| ATOM | 2553 | N   | GLY A | 320 | 10.531  | 80.058 | 14.100  | 1.00 | 39.74 |
| ATOM | 2554 | CA  | GLY A | 320 | 10.827  | 79.022 | 13.130  | 1.00 | 35.73 |
| ATOM | 2555 | C   | GLY A | 320 | 11. 611 | 79.582 | 11. 962 | 1.00 | 35.37 |
| ATOM | 2556 | O   | GLY A | 320 | 12.536  | 78.951 | 11.471  | 1.00 | 37.50 |
| ATOM | 2557 | N   | LEU A | 321 | 11. 270 | 80.786 | 11. 530 | 1.00 | 34.76 |
| ATOM | 2558 | CA  | LEU A | 321 | 11.967  | 81.393 | 10.415  | 1.00 | 39.63 |
| ATOM | 2559 | CB  | LEU A | 321 | 11.191  | 82.583 | 9.877   | 1.00 | 36.97 |
| ATOM | 2560 | CG  | LEU A | 321 | 9.901   | 82.168 | 9.187   | 1.00 | 38.18 |
| ATOM | 2561 | CD1 | LEU A | 321 | 9.271   | 83.392 | 8.570   | 1.00 | 38.33 |
| ATOM | 2562 | CD2 | LEU A | 321 | 10.181  | 81.108 | 8.134   | 1.00 | 35.19 |
| ATOM | 2563 | C   | LEU A | 321 | 13.382  | 81.805 | 10.757  | 1.00 | 44.08 |
| ATOM | 2564 | O   | LEU A | 321 | 14.287  | 81.606 | 9.953   | 1.00 | 46.65 |
| ATOM | 2565 | N   | VAL A | 322 | 13.581  | 82.378 | 11.941  | 1.00 | 49.49 |
| ATOM | 2566 | CA  | VAL A | 322 | 14.923  | 82.806 | 12.345  | 1.00 | 53.83 |
| ATOM | 2567 | CB  | VAL A | 322 | 14.939  | 83.617 | 13.671  | 1.00 | 53.89 |
| ATOM | 2568 | CG1 | VAL A | 322 | 13.945  | 84.767 | 13.615  | 1.00 | 53.18 |
| ATOM | 2569 | CG2 | VAL A | 322 | 14.698  | 82.698 | 14.869  | 1.00 | 55.17 |
| ATOM | 2570 | C   | VAL A | 322 | 15.894  | 81.645 | 12.511  | 1.00 | 54.31 |
| ATOM | 2571 | O   | VAL A | 322 | 17.104  | 81.848 | 12.478  | 1.00 | 59.46 |
| ATOM | 2572 | N   | SER A | 323 | 15.378  | 80.452 | 12.773  | 1.00 | 52.61 |
| ATOM | 2573 | CA  | SER A | 323 | 16.254  | 79.309 | 12.940  | 1.00 | 53.68 |
| ATOM | 2574 | CB  | SER A | 323 | 15.480  | 78.096 | 13.468  | 1.00 | 55.08 |
| ATOM | 2575 | OG  | SER A | 323 | 14.499  | 77.644 | 12.551  | 1.00 | 52.98 |
| ATOM | 2576 | C   | SER A | 323 | 16.913  | 78.965 | 11.616  | 1.00 | 54.49 |
| ATOM | 2577 | O   | SER A | 323 | 18.061  | 78.523 | 11.584  | 1.00 | 58.60 |
| ATOM | 2578 | N   | LEU A | 324 | 16.194  | 79.186 | 10.522  | 1.00 | 55.84 |
| ATOM | 2579 | CA  | LEU A | 324 | 16.725  | 78.861 | 9.207   | 1.00 | 56.10 |
| ATOM | 2580 | CB  | LEU A | 324 | 15.596  | 78.485 | 8.229   | 1.00 | 52.73 |
| ATOM | 2581 | CG  | LEU A | 324 | 14.383  | 79.396 | 8.017   | 1.00 | 51.08 |
| ATOM | 2582 | CD1 | LEU A | 324 | 14.679  | 80.431 | 6.945   | 1.00 | 54.72 |
| ATOM | 2583 | CD2 | LEU A | 324 | 13.183  | 78.561 | 7.606   | 1.00 | 50.43 |
| ATOM | 2584 | C   | LEU A | 324 | 17.637  | 79.928 | 8.625   | 1.00 | 57.85 |
| ATOM | 2585 | O   | LEU A | 324 | 17.696  | 81.050 | 9.116   | 1.00 | 55.56 |
| ATOM | 2586 | N   | ILE A | 325 | 18.379  | 79.536 | 7.595   | 1.00 | 62.83 |
| ATOM | 2587 | CA  | ILE A | 325 | 19.307  | 80.428 | 6.910   | 1.00 | 64.52 |
| ATOM | 2588 | CB  | ILE A | 325 | 20.264  | 79.668 | 5.969   | 1.00 | 64.56 |
| ATOM | 2589 | CG2 | ILE A | 325 | 21.516  | 80.496 | 5.747   | 1.00 | 65.36 |
| ATOM | 2590 | CG1 | ILE A | 325 | 20.591  | 78.271 | 6.516   | 1.00 | 65.53 |
| ATOM | 2591 | CD1 | ILE A | 325 | 19.563  | 77.197 | 6.136   | 1.00 | 67.86 |
| ATOM | 2592 | C   | ILE A | 325 | 18.501  | 81.383 | 6.034   | 1.00 | 65.56 |
| ATOM | 2593 | O   | ILE A | 325 | 17.808  | 80.957 | 5.110   | 1.00 | 66.01 |
| ATOM | 2594 | N   | ASN A | 326 | 18.621  | 82.673 | 6.312   | 1.00 | 67.38 |
| ATOM | 2595 | CA  | ASN A | 326 | 17.899  | 83.696 | 5.559   | 1.00 | 68.33 |
| ATOM | 2596 | CB  | ASN A | 326 | 18.205  | 85.097 | 6.105   | 1.00 | 73.56 |
| ATOM | 2597 | CG  | ASN A | 326 | 17.632  | 85.325 | 7.495   | 1.00 | 78.94 |
| ATOM | 2598 | OD1 | ASN A | 326 | 17.224  | 84.386 | 8.171   | 1.00 | 83.34 |
| ATOM | 2599 | ND2 | ASN A | 326 | 17.590  | 86.582 | 7.920   | 1.00 | 79.40 |
| ATOM | 2600 | C   | ASN A | 326 | 18.169  | 83.663 | 4.068   | 1.00 | 65.53 |
| ATOM | 2601 | O   | ASN A | 326 | 17.254  | 83.861 | 3.274   | 1.00 | 67.11 |
| ATOM | 2602 | N   | LYS A | 327 | 19.413  | 83.404 | 3.681   | 1.00 | 59.01 |
| ATOM | 2603 | CA  | LYS A | 327 | 19.761  | 83.355 | 2.263   | 1.00 | 54.20 |
| ATOM | 2604 | CB  | LYS A | 327 | 21.277  | 83.218 | 2.095   | 1.00 | 53.73 |
| ATOM | 2605 | CG  | LYS A | 327 | 22.021  | 84.515 | 2.327   | 1.00 | 53.84 |
| ATOM | 2606 | CD  | LYS A | 327 | 23.511  | 84.317 | 2.266   | 1.00 | 60.90 |
| ATOM | 2607 | CE  | LYS A | 327 | 24.262  | 85.605 | 2.584   | 1.00 | 61.87 |
| ATOM | 2608 | NZ  | LYS A | 327 | 24.203  | 86.582 | 1.467   | 1.00 | 58.17 |
| ATOM | 2609 | C   | LYS A | 327 | 19.033  | 82.256 | 1.500   | 1.00 | 51.14 |
| ATOM | 2610 | O   | LYS A | 327 | 18.610  | 82.472 | 0.370   | 1.00 | 50.58 |
| ATOM | 2611 | N   | ASN A | 328 | 18.868  | 81.088 | 2.109   | 1.00 | 51.00 |
| ATOM | 2612 | CA  | ASN A | 328 | 18.186  | 79.980 | 1.439   | 1.00 | 56.30 |
| ATOM | 2613 | CB  | ASN A | 328 | 18.717  | 78.637 | 1.947   | 1.00 | 59.34 |
| ATOM | 2614 | CG  | ASN A | 328 | 20.104  | 78.345 | 1.410   | 1.00 | 62.04 |
| ATOM | 2615 | OD1 | ASN A | 328 | 21.052  | 79.056 | 1.725   | 1.00 | 64.52 |
| ATOM | 2616 | ND2 | ASN A | 328 | 20.226  | 77.327 | 0.562   | 1.00 | 65.59 |
| ATOM | 2617 | C   | ASN A | 328 | 16.657  | 80.013 | 1.498   | 1.00 | 56.83 |
| ATOM | 2618 | O   | ASN A | 328 | 15.976  | 79.760 | 0.505   | 1.00 | 57.74 |
| ATOM | 2619 | N   | GLY A | 329 | 16.117  | 80.291 | 2.684   | 1.00 | 59.02 |
| ATOM | 2620 | CA  | GLY A | 329 | 14.678  | 80.340 | 2.864   | 1.00 | 57.93 |
| ATOM | 2621 | C   | GLY A | 329 | 13.973  | 79.011 | 2.645   | 1.00 | 61.61 |
| ATOM | 2622 | O   | GLY A | 329 | 14.604  | 77.939 | 2.645   | 1.00 | 63.66 |
| ATOM | 2623 | N   | GLN A | 330 | 12.665  | 79.134 | 2.426   | 1.00 | 63.44 |
| ATOM | 2624 | CA  | GLN A | 330 | 11. 647 | 78.088 | 2.186   | 1.00 | 62.51 |

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|      |      |     |       |     |        |        |        |      |       |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|
| ATOM | 2625 | CB  | GLN A | 330 | 12.152 | 76.612 | 2.170  | 1.00 | 61.84 |
| ATOM | 2626 | CG  | GLN A | 330 | 11.146 | 75.609 | 1.460  | 1.00 | 62.53 |
| ATOM | 2627 | CD  | GLN A | 330 | 11.591 | 74.116 | 1.364  | 1.00 | 61.91 |
| ATOM | 2628 | OE1 | GLN A | 330 | 10.948 | 73.200 | 1.946  | 1.00 | 56.42 |
| ATOM | 2629 | NE2 | GLN A | 330 | 12.658 | 73.864 | 0.605  | 1.00 | 56.02 |
| ATOM | 2630 | C   | GLN A | 330 | 10.703 | 78.366 | 3.357  | 1.00 | 61.76 |
| ATOM | 2631 | O   | GLN A | 330 | 11.044 | 78.121 | 4.511  | 1.00 | 61.59 |
| ATOM | 2632 | N   | THR A | 331 | 9.623  | 79.069 | 3.018  | 1.00 | 61.83 |
| ATOM | 2633 | CA  | THR A | 331 | 8.542  | 79.549 | 3.891  | 1.00 | 57.39 |
| ATOM | 2634 | CB  | THR A | 331 | 9.685  | 79.154 | 5.400  | 1.00 | 46.65 |
| ATOM | 2635 | OG1 | THR A | 331 | 8.904  | 77.740 | 5.517  | 1.00 | 38.61 |
| ATOM | 2636 | CG2 | THR A | 331 | 7.378  | 79.483 | 6.144  | 1.00 | 48.69 |
| ATOM | 2637 | C   | THR A | 331 | 8.427  | 81.085 | 3.668  | 1.00 | 59.73 |
| ATOM | 2638 | O   | THR A | 331 | 8.586  | 81.496 | 2.495  | 1.00 | 55.52 |
| ATOM | 2639 | OT  | THR A | 331 | 8.131  | 81.869 | 4.601  | 1.00 | 62.34 |
| ATOM | 2640 | MN  | MN A  | 350 | 10.357 | 71.058 | 3.078  | 1.00 | 32.10 |
| ATOM | 2641 | MN  | MN A  | 351 | 16.765 | 98.946 | -5.069 | 1.00 | 40.69 |
| END  |      |     |       |     |        |        |        |      |       |

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Table 3

|        |        |          |          |          |         |        |          |          |          |
|--------|--------|----------|----------|----------|---------|--------|----------|----------|----------|
| CRYST1 | 46.800 | 71.500   | 101.000  | 90.00    | 90.00   | 90.00  | 0.000000 | 0.000000 | 0.000000 |
| SCALE1 |        | 0.021368 | 0.000000 | 0.000000 |         |        | 0.000000 | 0.000000 | 0.000000 |
| SCALE2 |        | 0.000000 | 0.013986 | 0.000000 |         |        | 0.000000 | 0.000000 | 0.000000 |
| SCALE3 |        | 0.000000 | 0.000000 | 0.009901 |         |        |          |          |          |
| ATOM   | 1      | C1       | ACV      | 1        | 17.235  | 36.323 | 5.699    | 1.00     | 7.93     |
| ATOM   | 2      | C2       | ACV      | 1        | 15.798  | 36.590 | 6.165    | 1.00     | 7.47     |
| ATOM   | 3      | C3       | ACV      | 1        | 15.215  | 37.802 | 5.425    | 1.00     | 6.42     |
| ATOM   | 4      | C4       | ACV      | 1        | 13.766  | 38.091 | 5.918    | 1.00     | 7.71     |
| ATOM   | 5      | C7       | ACV      | 1        | 13.330  | 39.380 | 5.168    | 1.00     | 8.43     |
| ATOM   | 6      | C10      | ACV      | 1        | 11.912  | 39.669 | 5.584    | 1.00     | 8.88     |
| ATOM   | 7      | N11      | ACV      | 1        | 10.931  | 39.447 | 4.714    | 1.00     | 6.98     |
| ATOM   | 8      | C12      | ACV      | 1        | 9.503   | 39.719 | 4.858    | 1.00     | 7.75     |
| ATOM   | 9      | C13      | ACV      | 1        | 8.767   | 38.397 | 4.657    | 1.00     | 7.09     |
| ATOM   | 10     | N14      | ACV      | 1        | 15.791  | 36.747 | 7.696    | 1.00     | 8.98     |
| ATOM   | 11     | O15      | ACV      | 1        | 11.566  | 40.061 | 6.715    | 1.00     | 11.68    |
| ATOM   | 12     | C16      | ACV      | 1        | 9.131   | 40.743 | 3.765    | 1.00     | 7.15     |
| ATOM   | 13     | S17      | ACV      | 1        | 9.513   | 40.068 | 2.102    | 1.00     | 8.44     |
| ATOM   | 14     | O18      | ACV      | 1        | 9.269   | 37.306 | 4.670    | 1.00     | 9.78     |
| ATOM   | 15     | O19      | ACV      | 1        | 18.173  | 36.442 | 6.549    | 1.00     | 8.96     |
| ATOM   | 16     | O20      | ACV      | 1        | 17.393  | 36.068 | 4.492    | 1.00     | 7.91     |
| ATOM   | 17     | N29      | ACV      | 1        | 7.424   | 38.510 | 4.604    | 1.00     | 9.16     |
| ATOM   | 18     | C30      | ACV      | 1        | 6.543   | 37.341 | 4.409    | 1.00     | 9.68     |
| ATOM   | 19     | C31      | ACV      | 1        | 5.317   | 37.433 | 5.318    | 1.00     | 10.48    |
| ATOM   | 20     | C32      | ACV      | 1        | 6.104   | 37.147 | 2.912    | 1.00     | 12.78    |
| ATOM   | 21     | C33      | ACV      | 1        | 7.348   | 36.829 | 2.039    | 1.00     | 11.31    |
| ATOM   | 22     | C37      | ACV      | 1        | 5.562   | 38.560 | 2.564    | 1.00     | 18.82    |
| ATOM   | 23     | O42      | ACV      | 1        | 5.240   | 38.298 | 6.210    | 1.00     | 10.58    |
| ATOM   | 24     | O43      | ACV      | 1        | 4.417   | 36.560 | 5.151    | 1.00     | 9.69     |
| ATOM   | 25     | S        | SUL      | 2        | 13.002  | 14.100 | 2.417    | 1.00     | 25.69    |
| ATOM   | 26     | O1       | SUL      | 2        | 13.804  | 14.598 | 3.492    | 1.00     | 32.83    |
| ATOM   | 27     | O2       | SUL      | 2        | 13.918  | 13.558 | 1.424    | 1.00     | 41.91    |
| ATOM   | 28     | O3       | SUL      | 2        | 12.155  | 13.073 | 2.934    | 1.00     | 30.42    |
| ATOM   | 29     | O4       | SUL      | 2        | 12.299  | 15.076 | 1.614    | 1.00     | 21.23    |
| ATOM   | 30     | FE       | IUM      | 1000     | 7.903   | 40.943 | 0.544    | 1.00     | 7.64     |
| ATOM   | 31     | N        | SER      | 3        | -15.013 | 47.966 | -1.402   | 1.00     | 42.72    |
| ATOM   | 32     | CA       | SER      | 3        | -14.317 | 46.679 | -1.445   | 1.00     | 39.06    |
| ATOM   | 33     | C        | SER      | 3        | -12.942 | 46.953 | -2.052   | 1.00     | 36.17    |
| ATOM   | 34     | O        | SER      | 3        | -12.712 | 48.077 | -2.493   | 1.00     | 41.73    |
| ATOM   | 35     | CB       | SER      | 3        | -14.951 | 45.513 | -2.197   | 1.00     | 42.74    |
| ATOM   | 36     | OG       | SER      | 3        | -14.920 | 45.578 | -3.613   | 1.00     | 52.50    |
| ATOM   | 37     | N        | VAL      | 4        | -12.127 | 45.917 | -2.096   | 1.00     | 33.45    |
| ATOM   | 38     | CA       | VAL      | 4        | -10.801 | 46.077 | -2.708   | 1.00     | 30.02    |
| ATOM   | 39     | C        | VAL      | 4        | -10.826 | 45.243 | -3.983   | 1.00     | 26.11    |
| ATOM   | 40     | O        | VAL      | 4        | -11.331 | 44.137 | -3.995   | 1.00     | 26.45    |
| ATOM   | 41     | CB       | VAL      | 4        | -9.693  | 45.600 | -1.751   | 1.00     | 32.20    |
| ATOM   | 42     | CG1      | VAL      | 4        | -8.324  | 45.544 | -2.407   | 1.00     | 31.47    |
| ATOM   | 43     | CG2      | VAL      | 4        | -9.619  | 46.380 | -0.434   | 1.00     | 39.65    |
| ATOM   | 44     | CB       | SER      | 5        | -9.685  | 46.084 | -7.342   | 1.00     | 28.73    |
| ATOM   | 45     | OG       | SER      | 5        | -10.494 | 46.429 | -8.413   | 1.00     | 43.87    |
| ATOM   | 46     | C        | SER      | 5        | -9.128  | 43.958 | -6.292   | 1.00     | 21.38    |
| ATOM   | 47     | O        | SER      | 5        | -8.126  | 44.094 | -5.558   | 1.00     | 17.45    |
| ATOM   | 48     | N        | SER      | 5        | -10.297 | 45.742 | -5.071   | 1.00     | 22.91    |
| ATOM   | 49     | CA       | SER      | 5        | -10.216 | 45.050 | -6.347   | 1.00     | 24.13    |
| ATOM   | 50     | N        | LYS      | 6        | -9.338  | 42.900 | -7.057   | 1.00     | 20.27    |
| ATOM   | 51     | CA       | LYS      | 6        | -8.400  | 41.770 | -7.199   | 1.00     | 18.92    |
| ATOM   | 52     | CB       | LYS      | 6        | -9.148  | 40.516 | -7.644   | 1.00     | 25.88    |
| ATOM   | 53     | CG       | LYS      | 6        | -8.452  | 39.606 | -8.620   | 1.00     | 33.15    |
| ATOM   | 54     | CD       | LYS      | 6        | -8.676  | 38.116 | -8.377   | 1.00     | 36.92    |
| ATOM   | 55     | CE       | LYS      | 6        | -9.217  | 37.434 | -9.627   | 1.00     | 40.48    |
| ATOM   | 56     | NZ       | LYS      | 6        | -10.331 | 38.278 | -10.180  | 1.00     | 49.46    |
| ATOM   | 57     | C        | LYS      | 6        | -7.302  | 42.178 | -8.167   | 1.00     | 16.57    |
| ATOM   | 58     | O        | LYS      | 6        | -7.476  | 42.719 | -9.294   | 1.00     | 19.33    |
| ATOM   | 59     | N        | ALA      | 7        | -6.060  | 41.933 | -7.756   | 1.00     | 13.66    |
| ATOM   | 60     | CA       | ALA      | 7        | -4.879  | 42.175 | -8.572   | 1.00     | 12.78    |
| ATOM   | 61     | CB       | ALA      | 7        | -3.616  | 42.083 | -7.716   | 1.00     | 14.08    |
| ATOM   | 62     | C        | ALA      | 7        | -4.803  | 41.135 | -9.678   | 1.00     | 12.30    |
| ATOM   | 63     | O        | ALA      | 7        | -5.069  | 39.957 | -9.497   | 1.00     | 13.11    |
| ATOM   | 64     | N        | ASN      | 8        | -4.325  | 41.585 | -10.844  | 1.00     | 15.13    |
| ATOM   | 65     | CA       | ASN      | 8        | -4.026  | 40.653 | -11.913  | 1.00     | 16.54    |
| ATOM   | 66     | CB       | ASN      | 8        | -3.650  | 41.448 | -13.197  | 1.00     | 24.27    |
| ATOM   | 67     | CG       | ASN      | 8        | -4.274  | 40.597 | -14.298  | 1.00     | 29.61    |
| ATOM   | 68     | OD1      | ASN      | 8        | -3.669  | 39.640 | -14.787  | 1.00     | 35.60    |
| ATOM   | 69     | ND2      | ASN      | 8        | -5.528  | 40.986 | -14.477  | 1.00     | 43.75    |

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|      |     |     |     |    |        |        |         |      |       |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|
| ATOM | 70  | C   | ASN | 8  | -2.738 | 39.882 | -11.623 | 1.00 | 13.63 |
| ATOM | 71  | O   | ASN | 8  | -1.648 | 40.451 | -11.691 | 1.00 | 16.79 |
| ATOM | 72  | N   | VAL | 9  | -2.918 | 38.611 | -11.303 | 1.00 | 11.43 |
| ATOM | 73  | CA  | VAL | 9  | -1.809 | 37.707 | -11.016 | 1.00 | 10.00 |
| ATOM | 74  | CB  | VAL | 9  | -1.770 | 37.383 | -9.522  | 1.00 | 10.55 |
| ATOM | 75  | CG1 | VAL | 9  | -0.548 | 36.537 | -9.229  | 1.00 | 10.77 |
| ATOM | 76  | CG2 | VAL | 9  | -1.726 | 38.675 | -8.725  | 1.00 | 11.32 |
| ATOM | 77  | C   | VAL | 9  | -1.955 | 36.422 | -11.845 | 1.00 | 10.66 |
| ATOM | 78  | O   | VAL | 9  | -2.621 | 35.466 | -11.464 | 1.00 | 14.19 |
| ATOM | 79  | N   | PRO | 10 | -1.385 | 36.425 | -13.059 | 1.00 | 9.44  |
| ATOM | 80  | CD  | PRO | 10 | -0.544 | 37.474 | -13.650 | 1.00 | 10.90 |
| ATOM | 81  | CA  | PRO | 10 | -1.565 | 35.299 | -13.942 | 1.00 | 10.48 |
| ATOM | 82  | CB  | PRO | 10 | -0.901 | 35.749 | -15.235 | 1.00 | 12.92 |
| ATOM | 83  | CG  | PRO | 10 | -0.067 | 36.924 | -14.937 | 1.00 | 15.89 |
| ATOM | 84  | C   | PRO | 10 | -0.883 | 34.026 | -13.444 | 1.00 | 9.89  |
| ATOM | 85  | O   | PRO | 10 | 0.125  | 34.091 | -12.734 | 1.00 | 10.22 |
| ATOM | 86  | N   | LYS | 11 | -1.414 | 32.896 | -13.847 | 1.00 | 9.52  |
| ATOM | 87  | CA  | LYS | 11 | -0.815 | 31.597 | -13.586 | 1.00 | 9.53  |
| ATOM | 88  | CB  | LYS | 11 | -1.885 | 30.560 | -13.230 | 1.00 | 12.58 |
| ATOM | 89  | CG  | LYS | 11 | -2.651 | 30.971 | -11.965 | 1.00 | 18.45 |
| ATOM | 90  | CD  | LYS | 11 | -3.746 | 30.048 | -11.504 | 1.00 | 23.78 |
| ATOM | 91  | CE  | LYS | 11 | -4.685 | 30.872 | -10.629 | 1.00 | 25.46 |
| ATOM | 92  | NZ  | LYS | 11 | -4.154 | 31.101 | -9.250  | 1.00 | 27.77 |
| ATOM | 93  | C   | LYS | 11 | 0.020  | 31.211 | -14.803 | 1.00 | 10.29 |
| ATOM | 94  | O   | LYS | 11 | -0.482 | 31.172 | -15.926 | 1.00 | 16.95 |
| ATOM | 95  | N   | ILE | 12 | 1.301  | 31.019 | -14.640 | 1.00 | 8.18  |
| ATOM | 96  | CA  | ILE | 12 | 2.214  | 30.697 | -15.742 | 1.00 | 8.29  |
| ATOM | 97  | CB  | ILE | 12 | 3.358  | 31.733 | -15.815 | 1.00 | 8.64  |
| ATOM | 98  | CG2 | ILE | 12 | 4.366  | 31.311 | -16.864 | 1.00 | 9.33  |
| ATOM | 99  | CG1 | ILE | 12 | 2.860  | 33.160 | -16.018 | 1.00 | 9.90  |
| ATOM | 100 | CD1 | ILE | 12 | 3.945  | 34.238 | -15.984 | 1.00 | 10.28 |
| ATOM | 101 | C   | ILE | 12 | 2.749  | 29.284 | -15.518 | 1.00 | 7.89  |
| ATOM | 102 | O   | ILE | 12 | 3.346  | 28.974 | -14.504 | 1.00 | 7.80  |
| ATOM | 103 | N   | ASP | 13 | 2.542  | 28.428 | -16.522 | 1.00 | 8.72  |
| ATOM | 104 | CA  | ASP | 13 | 3.109  | 27.068 | -16.533 | 1.00 | 8.16  |
| ATOM | 105 | CB  | ASP | 13 | 2.391  | 26.193 | -17.536 | 1.00 | 9.68  |
| ATOM | 106 | CG  | ASP | 13 | 2.947  | 24.828 | -17.728 | 1.00 | 11.65 |
| ATOM | 107 | OD1 | ASP | 13 | 4.047  | 24.478 | -17.257 | 1.00 | 10.88 |
| ATOM | 108 | OD2 | ASP | 13 | 2.283  | 24.013 | -18.401 | 1.00 | 19.22 |
| ATOM | 109 | C   | ASP | 13 | 4.601  | 27.248 | -16.838 | 1.00 | 7.72  |
| ATOM | 110 | O   | ASP | 13 | 5.005  | 27.527 | -17.990 | 1.00 | 9.02  |
| ATOM | 111 | N   | VAL | 14 | 5.413  | 26.983 | -15.825 | 1.00 | 8.27  |
| ATOM | 112 | CA  | VAL | 14 | 6.862  | 27.170 | -15.947 | 1.00 | 8.27  |
| ATOM | 113 | CB  | VAL | 14 | 7.453  | 27.766 | -14.680 | 1.00 | 8.09  |
| ATOM | 114 | CG1 | VAL | 14 | 6.890  | 29.164 | -14.465 | 1.00 | 9.81  |
| ATOM | 115 | CG2 | VAL | 14 | 7.298  | 26.882 | -13.458 | 1.00 | 8.58  |
| ATOM | 116 | C   | VAL | 14 | 7.592  | 25.910 | -16.328 | 1.00 | 8.98  |
| ATOM | 117 | O   | VAL | 14 | 8.815  | 25.950 | -16.464 | 1.00 | 10.04 |
| ATOM | 118 | N   | SER | 15 | 6.851  | 24.822 | -16.531 | 1.00 | 9.65  |
| ATOM | 119 | CA  | SER | 15 | 7.532  | 23.572 | -16.883 | 1.00 | 9.94  |
| ATOM | 120 | CB  | SER | 15 | 6.548  | 22.411 | -16.994 | 1.00 | 10.80 |
| ATOM | 121 | OG  | SER | 15 | 5.618  | 22.532 | -18.063 | 1.00 | 12.34 |
| ATOM | 122 | C   | SER | 15 | 8.469  | 23.599 | -18.070 | 1.00 | 9.33  |
| ATOM | 123 | O   | SER | 15 | 9.519  | 22.915 | -18.009 | 1.00 | 9.96  |
| ATOM | 124 | N   | PRO | 16 | 8.218  | 24.364 | -19.141 | 1.00 | 10.18 |
| ATOM | 125 | CD  | PRO | 16 | 7.026  | 25.108 | -19.546 | 1.00 | 9.79  |
| ATOM | 126 | CA  | PRO | 16 | 9.220  | 24.381 | -20.209 | 1.00 | 10.12 |
| ATOM | 127 | CB  | PRO | 16 | 8.629  | 25.357 | -21.226 | 1.00 | 10.60 |
| ATOM | 128 | CG  | PRO | 16 | 7.127  | 25.247 | -21.015 | 1.00 | 11.12 |
| ATOM | 129 | C   | PRO | 16 | 10.583 | 24.909 | -19.807 | 1.00 | 9.66  |
| ATOM | 130 | O   | PRO | 16 | 11.579 | 24.613 | -20.444 | 1.00 | 11.72 |
| ATOM | 131 | N   | LEU | 17 | 10.666 | 25.693 | -18.711 | 1.00 | 10.05 |
| ATOM | 132 | CA  | LEU | 17 | 11.949 | 26.232 | -18.288 | 1.00 | 10.06 |
| ATOM | 133 | CB  | LEU | 17 | 11.738 | 27.358 | -17.276 | 1.00 | 8.52  |
| ATOM | 134 | CG  | LEU | 17 | 10.992 | 28.598 | -17.808 | 1.00 | 9.04  |
| ATOM | 135 | CD1 | LEU | 17 | 10.784 | 29.540 | -16.622 | 1.00 | 9.12  |
| ATOM | 136 | CD2 | LEU | 17 | 11.738 | 29.314 | -18.922 | 1.00 | 10.89 |
| ATOM | 137 | C   | LEU | 17 | 12.890 | 25.183 | -17.692 | 1.00 | 11.62 |
| ATOM | 138 | O   | LEU | 17 | 14.087 | 25.442 | -17.466 | 1.00 | 12.52 |
| ATOM | 139 | N   | PHE | 18 | 12.403 | 23.970 | -17.499 | 1.00 | 11.77 |
| ATOM | 140 | CA  | PHE | 18 | 13.234 | 22.862 | -17.065 | 1.00 | 12.92 |
| ATOM | 141 | CB  | PHE | 18 | 12.363 | 21.947 | -16.180 | 1.00 | 12.94 |
| ATOM | 142 | CG  | PHE | 18 | 12.070 | 22.571 | -14.820 | 1.00 | 13.53 |

|      |     |     |     |    |        |        |         |      |       |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|
| ATOM | 143 | CD1 | PHE | 18 | 10.872 | 23.207 | -14.598 | 1.00 | 17.84 |
| ATOM | 144 | CD2 | PHE | 18 | 12.965 | 22.503 | -13.766 | 1.00 | 14.00 |
| ATOM | 145 | CE1 | PHE | 18 | 10.537 | 23.720 | -13.359 | 1.00 | 17.86 |
| ATOM | 146 | CE2 | PHE | 18 | 12.638 | 22.974 | -12.519 | 1.00 | 14.38 |
| ATOM | 147 | CZ  | PHE | 18 | 11.444 | 23.614 | -12.326 | 1.00 | 15.20 |
| ATOM | 148 | C   | PHE | 18 | 13.768 | 22.054 | -18.231 | 1.00 | 14.72 |
| ATOM | 149 | O   | PHE | 18 | 14.567 | 21.129 | -18.012 | 1.00 | 17.55 |
| ATOM | 150 | N   | GLY | 19 | 13.321 | 22.349 | -19.445 | 1.00 | 15.60 |
| ATOM | 151 | CA  | GLY | 19 | 13.718 | 21.513 | -20.583 | 1.00 | 17.05 |
| ATOM | 152 | C   | GLY | 19 | 14.489 | 22.248 | -21.663 | 1.00 | 16.88 |
| ATOM | 153 | O   | GLY | 19 | 15.092 | 23.280 | -21.384 | 1.00 | 16.84 |
| ATOM | 154 | N   | ASP | 20 | 14.471 | 21.679 | -22.868 | 1.00 | 18.23 |
| ATOM | 155 | CA  | ASP | 20 | 15.241 | 22.147 | -23.997 | 1.00 | 19.57 |
| ATOM | 156 | C   | ASP | 20 | 14.418 | 22.595 | -25.186 | 1.00 | 16.96 |
| ATOM | 157 | O   | ASP | 20 | 14.976 | 22.646 | -26.285 | 1.00 | 18.78 |
| ATOM | 158 | CB  | ASP | 20 | 16.172 | 21.025 | -24.491 | 1.00 | 25.96 |
| ATOM | 159 | CG  | ASP | 20 | 16.954 | 20.446 | -23.320 | 1.00 | 30.78 |
| ATOM | 160 | OD1 | ASP | 20 | 17.102 | 19.208 | -23.399 | 1.00 | 38.92 |
| ATOM | 161 | OD2 | ASP | 20 | 17.315 | 21.213 | -22.393 | 1.00 | 40.12 |
| ATOM | 162 | N   | ASP | 21 | 13.161 | 22.913 | -25.013 | 1.00 | 16.58 |
| ATOM | 163 | CA  | ASP | 21 | 12.383 | 23.435 | -26.145 | 1.00 | 16.91 |
| ATOM | 164 | CB  | ASP | 21 | 10.920 | 23.028 | -25.985 | 1.00 | 18.23 |
| ATOM | 165 | CG  | ASP | 21 | 10.023 | 23.362 | -27.142 | 1.00 | 20.86 |
| ATOM | 166 | OD1 | ASP | 21 | 10.313 | 24.380 | -27.796 | 1.00 | 21.70 |
| ATOM | 167 | OD2 | ASP | 21 | 8.968  | 22.756 | -27.430 | 1.00 | 27.79 |
| ATOM | 168 | C   | ASP | 21 | 12.561 | 24.961 | -26.116 | 1.00 | 14.20 |
| ATOM | 169 | O   | ASP | 21 | 11.892 | 25.648 | -25.343 | 1.00 | 12.84 |
| ATOM | 170 | N   | GLN | 22 | 13.504 | 25.500 | -26.887 | 1.00 | 15.68 |
| ATOM | 171 | CA  | GLN | 22 | 13.813 | 26.915 | -26.764 | 1.00 | 13.82 |
| ATOM | 172 | CB  | GLN | 22 | 15.048 | 27.347 | -27.545 | 1.00 | 13.58 |
| ATOM | 173 | CG  | GLN | 22 | 16.257 | 26.474 | -27.348 | 1.00 | 15.37 |
| ATOM | 174 | CD  | GLN | 22 | 16.663 | 26.189 | -25.918 | 1.00 | 16.56 |
| ATOM | 175 | OE1 | GLN | 22 | 16.485 | 27.042 | -25.067 | 1.00 | 19.01 |
| ATOM | 176 | NE2 | GLN | 22 | 17.205 | 24.984 | -25.728 | 1.00 | 19.39 |
| ATOM | 177 | C   | GLN | 22 | 12.654 | 27.819 | -27.116 | 1.00 | 13.52 |
| ATOM | 178 | O   | GLN | 22 | 12.484 | 28.853 | -26.449 | 1.00 | 11.96 |
| ATOM | 179 | N   | ALA | 23 | 11.890 | 27.480 | -28.125 | 1.00 | 16.53 |
| ATOM | 180 | CA  | ALA | 23 | 10.739 | 28.320 | -28.488 | 1.00 | 16.41 |
| ATOM | 181 | CB  | ALA | 23 | 10.088 | 27.855 | -29.796 | 1.00 | 22.56 |
| ATOM | 182 | C   | ALA | 23 | 9.715  | 28.331 | -27.352 | 1.00 | 13.99 |
| ATOM | 183 | O   | ALA | 23 | 9.120  | 29.380 | -27.065 | 1.00 | 13.68 |
| ATOM | 184 | N   | ALA | 24 | 9.451  | 27.160 | -26.761 | 1.00 | 13.08 |
| ATOM | 185 | CA  | ALA | 24 | 8.481  | 27.122 | -25.650 | 1.00 | 11.55 |
| ATOM | 186 | CB  | ALA | 24 | 8.214  | 25.694 | -25.217 | 1.00 | 13.62 |
| ATOM | 187 | C   | ALA | 24 | 8.988  | 27.977 | -24.524 | 1.00 | 9.62  |
| ATOM | 188 | O   | ALA | 24 | 8.213  | 28.627 | -23.815 | 1.00 | 9.80  |
| ATOM | 189 | N   | LYS | 25 | 10.278 | 27.958 | -24.263 | 1.00 | 10.01 |
| ATOM | 190 | CA  | LYS | 25 | 10.844 | 28.781 | -23.178 | 1.00 | 9.16  |
| ATOM | 191 | CB  | LYS | 25 | 12.332 | 28.472 | -23.004 | 1.00 | 9.87  |
| ATOM | 192 | CG  | LYS | 25 | 12.600 | 27.128 | -22.327 | 1.00 | 13.94 |
| ATOM | 193 | CD  | LYS | 25 | 14.077 | 27.106 | -21.852 | 1.00 | 21.25 |
| ATOM | 194 | CE  | LYS | 25 | 14.817 | 25.974 | -22.406 | 1.00 | 24.07 |
| ATOM | 195 | NZ  | LYS | 25 | 16.254 | 26.073 | -22.150 | 1.00 | 19.05 |
| ATOM | 196 | C   | LYS | 25 | 10.657 | 30.249 | -23.474 | 1.00 | 7.92  |
| ATOM | 197 | O   | LYS | 25 | 10.375 | 31.042 | -22.566 | 1.00 | 8.19  |
| ATOM | 198 | N   | MET | 26 | 10.811 | 30.662 | -24.728 | 1.00 | 8.75  |
| ATOM | 199 | CA  | MET | 26 | 10.564 | 32.085 | -25.068 | 1.00 | 9.12  |
| ATOM | 200 | CB  | MET | 26 | 10.903 | 32.408 | -26.546 | 1.00 | 9.73  |
| ATOM | 201 | CG  | MET | 26 | 12.399 | 32.424 | -26.816 | 1.00 | 10.03 |
| ATOM | 202 | SD  | MET | 26 | 13.322 | 33.724 | -25.970 | 1.00 | 10.21 |
| ATOM | 203 | CE  | MET | 26 | 13.056 | 35.132 | -27.066 | 1.00 | 10.95 |
| ATOM | 204 | C   | MET | 26 | 9.115  | 32.487 | -24.804 | 1.00 | 8.72  |
| ATOM | 205 | O   | MET | 26 | 8.828  | 33.594 | -24.356 | 1.00 | 8.27  |
| ATOM | 206 | N   | ARG | 27 | 8.163  | 31.585 | -25.091 | 1.00 | 8.42  |
| ATOM | 207 | CA  | ARG | 27 | 6.767  | 31.903 | -24.809 | 1.00 | 9.14  |
| ATOM | 208 | CB  | ARG | 27 | 5.842  | 30.894 | -25.505 | 1.00 | 10.27 |
| ATOM | 209 | CG  | ARG | 27 | 5.895  | 31.042 | -27.031 | 1.00 | 11.63 |
| ATOM | 210 | CD  | ARG | 27 | 4.969  | 30.149 | -27.808 | 1.00 | 15.41 |
| ATOM | 211 | NE  | ARG | 27 | 5.322  | 28.732 | -27.657 | 1.00 | 17.68 |
| ATOM | 212 | CZ  | ARG | 27 | 5.998  | 28.016 | -28.551 | 1.00 | 17.12 |
| ATOM | 213 | NH1 | ARG | 27 | 6.271  | 26.720 | -28.347 | 1.00 | 18.08 |
| ATOM | 214 | NH2 | ARG | 27 | 6.357  | 28.591 | -29.680 | 1.00 | 19.32 |
| ATOM | 215 | C   | ARG | 27 | 6.496  | 32.020 | -23.319 | 1.00 | 9.48  |

|      |     |     |     |    |        |        |         |      |       |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|
| ATOM | 216 | O   | ARG | 27 | 5.649  | 32.854 | -22.925 | 1.00 | 9.79  |
| ATOM | 217 | N   | VAL | 28 | 7.214  | 31.249 | -22.488 | 1.00 | 7.80  |
| ATOM | 218 | CA  | VAL | 28 | 7.129  | 31.447 | -21.039 | 1.00 | 7.80  |
| ATOM | 219 | CB  | VAL | 28 | 7.799  | 30.307 | -20.275 | 1.00 | 8.02  |
| ATOM | 220 | CG1 | VAL | 28 | 7.803  | 30.582 | -18.782 | 1.00 | 9.37  |
| ATOM | 221 | CG2 | VAL | 28 | 7.184  | 28.970 | -20.553 | 1.00 | 10.98 |
| ATOM | 222 | C   | VAL | 28 | 7.743  | 32.786 | -20.643 | 1.00 | 7.31  |
| ATOM | 223 | O   | VAL | 28 | 7.164  | 33.556 | -19.853 | 1.00 | 7.76  |
| ATOM | 224 | N   | ALA | 29 | 8.909  | 33.096 | -21.235 | 1.00 | 7.04  |
| ATOM | 225 | CA  | ALA | 29 | 9.578  | 34.368 | -20.949 | 1.00 | 7.37  |
| ATOM | 226 | CB  | ALA | 29 | 10.870 | 34.447 | -21.743 | 1.00 | 7.98  |
| ATOM | 227 | C   | ALA | 29 | 8.691  | 35.579 | -21.233 | 1.00 | 7.31  |
| ATOM | 228 | O   | ALA | 29 | 8.662  | 36.547 | -20.478 | 1.00 | 8.13  |
| ATOM | 229 | N   | GLN | 30 | 7.902  | 35.483 | -22.319 | 1.00 | 7.11  |
| ATOM | 230 | CA  | GLN | 30 | 7.001  | 36.576 | -22.637 | 1.00 | 7.56  |
| ATOM | 231 | CB  | GLN | 30 | 6.261  | 36.323 | -23.976 | 1.00 | 8.19  |
| ATOM | 232 | CG  | GLN | 30 | 5.378  | 37.456 | -24.427 | 1.00 | 8.58  |
| ATOM | 233 | CD  | GLN | 30 | 3.966  | 37.535 | -23.845 | 1.00 | 8.95  |
| ATOM | 234 | OE1 | GLN | 30 | 3.396  | 36.491 | -23.534 | 1.00 | 10.78 |
| ATOM | 235 | NE2 | GLN | 30 | 3.570  | 38.741 | -23.481 | 1.00 | 9.99  |
| ATOM | 236 | C   | GLN | 30 | 6.005  | 36.784 | -21.497 | 1.00 | 6.94  |
| ATOM | 237 | O   | GLN | 30 | 5.631  | 37.936 | -21.231 | 1.00 | 8.27  |
| ATOM | 238 | N   | GLN | 31 | 5.464  | 35.677 | -20.996 | 1.00 | 7.41  |
| ATOM | 239 | CA  | GLN | 31 | 4.470  | 35.750 | -19.933 | 1.00 | 7.30  |
| ATOM | 240 | CB  | GLN | 31 | 3.924  | 34.357 | -19.675 | 1.00 | 8.13  |
| ATOM | 241 | CG  | GLN | 31 | 3.117  | 33.748 | -20.829 | 1.00 | 9.37  |
| ATOM | 242 | CD  | GLN | 31 | 2.722  | 32.316 | -20.493 | 1.00 | 11.83 |
| ATOM | 243 | OE1 | GLN | 31 | 1.843  | 32.090 | -19.656 | 1.00 | 15.21 |
| ATOM | 244 | NE2 | GLN | 31 | 3.391  | 31.367 | -21.108 | 1.00 | 18.42 |
| ATOM | 245 | C   | GLN | 31 | 5.093  | 36.370 | -18.681 | 1.00 | 7.43  |
| ATOM | 246 | O   | GLN | 31 | 4.459  | 37.197 | -18.024 | 1.00 | 7.98  |
| ATOM | 247 | N   | ILE | 32 | 6.326  | 36.030 | -18.367 | 1.00 | 6.96  |
| ATOM | 248 | CA  | ILE | 32 | 7.047  | 36.640 | -17.258 | 1.00 | 7.29  |
| ATOM | 249 | CB  | ILE | 32 | 8.389  | 35.925 | -17.010 | 1.00 | 7.37  |
| ATOM | 250 | CG2 | ILE | 32 | 9.254  | 36.685 | -16.004 | 1.00 | 9.11  |
| ATOM | 251 | CG1 | ILE | 32 | 8.126  | 34.504 | -16.497 | 1.00 | 7.84  |
| ATOM | 252 | CD1 | ILE | 32 | 9.335  | 33.611 | -16.390 | 1.00 | 9.10  |
| ATOM | 253 | C   | ILE | 32 | 7.235  | 38.139 | -17.496 | 1.00 | 7.13  |
| ATOM | 254 | O   | ILE | 32 | 7.023  | 38.945 | -16.602 | 1.00 | 8.31  |
| ATOM | 255 | N   | ASP | 33 | 7.632  | 38.515 | -18.717 | 1.00 | 7.76  |
| ATOM | 256 | CA  | ASP | 33 | 7.801  | 39.927 | -19.072 | 1.00 | 8.04  |
| ATOM | 257 | CB  | ASP | 33 | 8.257  | 40.026 | -20.550 | 1.00 | 8.19  |
| ATOM | 258 | CG  | ASP | 33 | 8.447  | 41.482 | -20.994 | 1.00 | 8.88  |
| ATOM | 259 | OD1 | ASP | 33 | 9.429  | 42.118 | -20.550 | 1.00 | 9.63  |
| ATOM | 260 | OD2 | ASP | 33 | 7.560  | 41.941 | -21.792 | 1.00 | 9.07  |
| ATOM | 261 | C   | ASP | 33 | 6.480  | 40.675 | -18.835 | 1.00 | 7.95  |
| ATOM | 262 | O   | ASP | 33 | 6.480  | 41.751 | -18.200 | 1.00 | 8.54  |
| ATOM | 263 | N   | ALA | 34 | 5.357  | 40.154 | -19.355 | 1.00 | 8.10  |
| ATOM | 264 | CA  | ALA | 34 | 4.079  | 40.834 | -19.202 | 1.00 | 8.69  |
| ATOM | 265 | CB  | ALA | 34 | 2.993  | 40.062 | -19.938 | 1.00 | 9.24  |
| ATOM | 266 | C   | ALA | 34 | 3.709  | 41.028 | -17.735 | 1.00 | 8.36  |
| ATOM | 267 | O   | ALA | 34 | 3.284  | 42.105 | -17.299 | 1.00 | 9.82  |
| ATOM | 268 | N   | ALA | 35 | 3.903  | 39.967 | -16.933 | 1.00 | 8.64  |
| ATOM | 269 | CA  | ALA | 35 | 3.505  | 40.093 | -15.538 | 1.00 | 9.10  |
| ATOM | 270 | CB  | ALA | 35 | 3.527  | 38.723 | -14.870 | 1.00 | 11.05 |
| ATOM | 271 | C   | ALA | 35 | 4.423  | 41.047 | -14.779 | 1.00 | 9.17  |
| ATOM | 272 | O   | ALA | 35 | 3.968  | 41.822 | -13.942 | 1.00 | 10.62 |
| ATOM | 273 | N   | SER | 36 | 5.709  | 41.042 | -15.146 | 1.00 | 8.20  |
| ATOM | 274 | CA  | SER | 36 | 6.683  | 41.896 | -14.467 | 1.00 | 7.99  |
| ATOM | 275 | CB  | SER | 36 | 8.108  | 41.485 | -14.830 | 1.00 | 8.90  |
| ATOM | 276 | OG  | SER | 36 | 8.354  | 40.129 | -14.485 | 1.00 | 8.75  |
| ATOM | 277 | C   | SER | 36 | 6.436  | 43.364 | -14.801 | 1.00 | 9.43  |
| ATOM | 278 | O   | SER | 36 | 6.761  | 44.224 | -13.994 | 1.00 | 12.45 |
| ATOM | 279 | N   | ARG | 37 | 5.871  | 43.633 | -15.993 | 1.00 | 9.00  |
| ATOM | 280 | CA  | ARG | 37 | 5.572  | 44.996 | -16.415 | 1.00 | 10.53 |
| ATOM | 281 | CB  | ARG | 37 | 5.685  | 45.095 | -17.931 | 1.00 | 11.22 |
| ATOM | 282 | CG  | ARG | 37 | 7.046  | 44.858 | -18.544 | 1.00 | 12.00 |
| ATOM | 283 | CD  | ARG | 37 | 7.074  | 44.615 | -20.051 | 1.00 | 14.37 |
| ATOM | 284 | NE  | ARG | 37 | 6.514  | 45.706 | -20.881 | 1.00 | 15.54 |
| ATOM | 285 | CZ  | ARG | 37 | 6.327  | 45.575 | -22.190 | 1.00 | 15.00 |
| ATOM | 286 | NH1 | ARG | 37 | 6.682  | 44.430 | -22.781 | 1.00 | 16.31 |
| ATOM | 287 | NH2 | ARG | 37 | 5.812  | 46.595 | -22.875 | 1.00 | 14.87 |
| ATOM | 288 | C   | ARG | 37 | 4.204  | 45.459 | -15.925 | 1.00 | 11.82 |

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|      |     |     |     |    |        |        |         |      |       |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|
| ATOM | 289 | O   | ARG | 37 | 3.914  | 46.654 | -15.947 | 1.00 | 17.60 |
| ATOM | 290 | N   | ASP | 38 | 3.367  | 44.520 | -15.475 | 1.00 | 12.19 |
| ATOM | 291 | CA  | ASP | 38 | 2.045  | 44.889 | -14.976 | 1.00 | 14.66 |
| ATOM | 292 | CB  | ASP | 38 | 1.017  | 43.860 | -15.463 | 1.00 | 16.65 |
| ATOM | 293 | CG  | ASP | 38 | -0.441 | 44.105 | -15.173 | 1.00 | 17.06 |
| ATOM | 294 | OD1 | ASP | 38 | -0.763 | 45.278 | -14.922 | 1.00 | 22.39 |
| ATOM | 295 | OD2 | ASP | 38 | -1.316 | 43.219 | -15.263 | 1.00 | 20.09 |
| ATOM | 296 | C   | ASP | 38 | 2.102  | 45.018 | -13.455 | 1.00 | 13.71 |
| ATOM | 297 | O   | ASP | 38 | 2.736  | 45.927 | -12.904 | 1.00 | 14.27 |
| ATOM | 298 | N   | THR | 39 | 1.460  | 44.073 | -12.737 | 1.00 | 11.56 |
| ATOM | 299 | CA  | THR | 39 | 1.415  | 44.205 | -11.298 | 1.00 | 11.81 |
| ATOM | 300 | CB  | THR | 39 | 0.320  | 43.390 | -10.584 | 1.00 | 14.06 |
| ATOM | 301 | OG1 | THR | 39 | 0.687  | 41.990 | -10.698 | 1.00 | 17.03 |
| ATOM | 302 | CG2 | THR | 39 | -1.008 | 43.691 | -11.223 | 1.00 | 17.60 |
| ATOM | 303 | C   | THR | 39 | 2.721  | 43.776 | -10.634 | 1.00 | 10.17 |
| ATOM | 304 | O   | THR | 39 | 2.920  | 44.118 | -9.459  | 1.00 | 11.25 |
| ATOM | 305 | N   | GLY | 40 | 3.510  | 42.982 | -11.367 | 1.00 | 9.14  |
| ATOM | 306 | CA  | GLY | 40 | 4.740  | 42.526 | -10.777 | 1.00 | 8.52  |
| ATOM | 307 | C   | GLY | 40 | 4.618  | 41.178 | -10.115 | 1.00 | 9.63  |
| ATOM | 308 | O   | GLY | 40 | 5.587  | 40.753 | -9.505  | 1.00 | 14.89 |
| ATOM | 309 | N   | PHE | 41 | 3.477  | 40.522 | -10.124 | 1.00 | 8.18  |
| ATOM | 310 | CA  | PHE | 41 | 3.307  | 39.207 | -9.532  | 1.00 | 7.48  |
| ATOM | 311 | CB  | PHE | 41 | 2.353  | 39.290 | -8.343  | 1.00 | 7.50  |
| ATOM | 312 | CG  | PHE | 41 | 2.952  | 39.927 | -7.078  | 1.00 | 7.93  |
| ATOM | 313 | CD1 | PHE | 41 | 2.936  | 41.286 | -6.859  | 1.00 | 8.43  |
| ATOM | 314 | CD2 | PHE | 41 | 3.499  | 39.110 | -6.100  | 1.00 | 7.47  |
| ATOM | 315 | CE1 | PHE | 41 | 3.446  | 41.812 | -5.683  | 1.00 | 8.79  |
| ATOM | 316 | CE2 | PHE | 41 | 4.040  | 39.635 | -4.933  | 1.00 | 8.21  |
| ATOM | 317 | CZ  | PHE | 41 | 4.032  | 40.998 | -4.757  | 1.00 | 8.46  |
| ATOM | 318 | C   | PHE | 41 | 2.782  | 38.226 | -10.550 | 1.00 | 6.88  |
| ATOM | 319 | O   | PHE | 41 | 1.952  | 38.554 | -11.401 | 1.00 | 9.03  |
| ATOM | 320 | N   | PHE | 42 | 3.164  | 36.978 | -10.374 | 1.00 | 6.68  |
| ATOM | 321 | CA  | PHE | 42 | 2.539  | 35.845 | -11.075 | 1.00 | 6.92  |
| ATOM | 322 | CB  | PHE | 42 | 3.148  | 35.586 | -12.456 | 1.00 | 7.96  |
| ATOM | 323 | CG  | PHE | 42 | 4.564  | 35.072 | -12.516 | 1.00 | 7.35  |
| ATOM | 324 | CD1 | PHE | 42 | 4.802  | 33.699 | -12.586 | 1.00 | 7.79  |
| ATOM | 325 | CD2 | PHE | 42 | 5.637  | 35.931 | -12.518 | 1.00 | 8.85  |
| ATOM | 326 | CE1 | PHE | 42 | 6.124  | 33.266 | -12.696 | 1.00 | 8.64  |
| ATOM | 327 | CE2 | PHE | 42 | 6.951  | 35.498 | -12.656 | 1.00 | 9.37  |
| ATOM | 328 | CZ  | PHE | 42 | 7.193  | 34.141 | -12.740 | 1.00 | 9.28  |
| ATOM | 329 | C   | PHE | 42 | 2.620  | 34.594 | -10.216 | 1.00 | 6.60  |
| ATOM | 330 | O   | PHE | 42 | 3.489  | 34.518 | -9.338  | 1.00 | 6.98  |
| ATOM | 331 | N   | TYR | 43 | 1.783  | 33.606 | -10.477 | 1.00 | 6.57  |
| ATOM | 332 | CA  | TYR | 43 | 1.913  | 32.290 | -9.860  | 1.00 | 6.96  |
| ATOM | 333 | CB  | TYR | 43 | 0.575  | 31.694 | -9.466  | 1.00 | 7.72  |
| ATOM | 334 | CG  | TYR | 43 | 0.098  | 32.111 | -8.088  | 1.00 | 7.41  |
| ATOM | 335 | CD1 | TYR | 43 | -0.901 | 33.078 | -7.938  | 1.00 | 8.92  |
| ATOM | 336 | CE1 | TYR | 43 | -1.335 | 33.480 | -6.697  | 1.00 | 9.19  |
| ATOM | 337 | CD2 | TYR | 43 | 0.664  | 31.618 | -6.939  | 1.00 | 7.76  |
| ATOM | 338 | CE2 | TYR | 43 | 0.248  | 32.035 | -5.690  | 1.00 | 8.82  |
| ATOM | 339 | CZ  | TYR | 43 | -0.715 | 32.992 | -5.574  | 1.00 | 9.99  |
| ATOM | 340 | OH  | TYR | 43 | -1.130 | 33.349 | -4.303  | 1.00 | 11.00 |
| ATOM | 341 | C   | TYR | 43 | 2.625  | 31.390 | -10.867 | 1.00 | 6.77  |
| ATOM | 342 | O   | TYR | 43 | 2.160  | 31.203 | -11.985 | 1.00 | 9.17  |
| ATOM | 343 | N   | ALA | 44 | 3.663  | 30.736 | -10.386 | 1.00 | 6.74  |
| ATOM | 344 | CA  | ALA | 44 | 4.321  | 29.654 | -11.138 | 1.00 | 6.80  |
| ATOM | 345 | CB  | ALA | 44 | 5.766  | 29.522 | -10.683 | 1.00 | 6.89  |
| ATOM | 346 | C   | ALA | 44 | 3.590  | 28.345 | -10.834 | 1.00 | 6.81  |
| ATOM | 347 | O   | ALA | 44 | 3.423  | 27.965 | -9.679  | 1.00 | 7.69  |
| ATOM | 348 | N   | VAL | 45 | 3.075  | 27.695 | -11.849 | 1.00 | 7.45  |
| ATOM | 349 | CA  | VAL | 45 | 2.373  | 26.431 | -11.766 | 1.00 | 7.41  |
| ATOM | 350 | CB  | VAL | 45 | 0.902  | 26.570 | -12.161 | 1.00 | 9.68  |
| ATOM | 351 | CG1 | VAL | 45 | 0.228  | 27.601 | -11.255 | 1.00 | 10.94 |
| ATOM | 352 | CG2 | VAL | 45 | 0.670  | 26.895 | -13.632 | 1.00 | 10.29 |
| ATOM | 353 | C   | VAL | 45 | 3.120  | 25.384 | -12.583 | 1.00 | 7.22  |
| ATOM | 354 | O   | VAL | 45 | 3.984  | 25.718 | -13.393 | 1.00 | 7.51  |
| ATOM | 355 | N   | ASN | 46 | 2.862  | 24.095 | -12.325 | 1.00 | 8.30  |
| ATOM | 356 | CA  | ASN | 46 | 3.565  | 22.985 | -12.948 | 1.00 | 8.32  |
| ATOM | 357 | CB  | ASN | 46 | 3.323  | 22.885 | -14.449 | 1.00 | 11.81 |
| ATOM | 358 | CG  | ASN | 46 | 1.875  | 22.704 | -14.786 | 1.00 | 18.20 |
| ATOM | 359 | OD1 | ASN | 46 | 1.395  | 21.610 | -14.470 | 1.00 | 31.96 |
| ATOM | 360 | ND2 | ASN | 46 | 1.269  | 23.750 | -15.306 | 1.00 | 24.56 |
| ATOM | 361 | C   | ASN | 46 | 5.043  | 23.111 | -12.634 | 1.00 | 8.17  |

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|      |     |     |     |    |        |        |         |      |       |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|
| ATOM | 362 | O   | ASN | 46 | 5.936  | 22.860 | -13.449 | 1.00 | 10.28 |
| ATOM | 363 | N   | HIS | 47 | 5.323  | 23.425 | -11.366 | 1.00 | 8.42  |
| ATOM | 364 | CA  | HIS | 47 | 6.663  | 23.646 | -10.843 | 1.00 | 8.14  |
| ATOM | 365 | CB  | HIS | 47 | 6.618  | 24.724 | -9.775  | 1.00 | 8.35  |
| ATOM | 366 | CG  | HIS | 47 | 5.590  | 24.430 | -8.727  | 1.00 | 7.34  |
| ATOM | 367 | CD2 | HIS | 47 | 4.399  | 25.000 | -8.504  | 1.00 | 7.88  |
| ATOM | 368 | ND1 | HIS | 47 | 5.719  | 23.383 | -7.812  | 1.00 | 7.39  |
| ATOM | 369 | CE1 | HIS | 47 | 4.626  | 23.360 | -7.052  | 1.00 | 8.04  |
| ATOM | 370 | NE2 | HIS | 47 | 3.827  | 24.344 | -7.440  | 1.00 | 8.14  |
| ATOM | 371 | C   | HIS | 47 | 7.375  | 22.430 | -10.325 | 1.00 | 7.89  |
| ATOM | 372 | O   | HIS | 47 | 8.580  | 22.464 | -10.091 | 1.00 | 9.85  |
| ATOM | 373 | N   | GLY | 48 | 6.691  | 21.328 | -10.139 | 1.00 | 8.33  |
| ATOM | 374 | CA  | GLY | 48 | 7.238  | 20.053 | -9.749  | 1.00 | 8.83  |
| ATOM | 375 | C   | GLY | 48 | 7.522  | 19.849 | -8.282  | 1.00 | 8.46  |
| ATOM | 376 | O   | GLY | 48 | 8.060  | 18.780 | -7.953  | 1.00 | 11.24 |
| ATOM | 377 | N   | ILE | 49 | 7.267  | 20.817 | -7.412  | 1.00 | 7.06  |
| ATOM | 378 | CA  | ILE | 49 | 7.568  | 20.636 | -6.015  | 1.00 | 6.70  |
| ATOM | 379 | CB  | ILE | 49 | 8.093  | 21.962 | -5.389  | 1.00 | 7.04  |
| ATOM | 380 | CG2 | ILE | 49 | 8.286  | 21.829 | -3.886  | 1.00 | 7.67  |
| ATOM | 381 | CG1 | ILE | 49 | 9.383  | 22.383 | -6.077  | 1.00 | 8.13  |
| ATOM | 382 | CD1 | ILE | 49 | 9.964  | 23.699 | -5.584  | 1.00 | 9.61  |
| ATOM | 383 | C   | ILE | 49 | 6.327  | 20.166 | -5.245  | 1.00 | 6.55  |
| ATOM | 384 | O   | ILE | 49 | 5.210  | 20.605 | -5.497  | 1.00 | 7.34  |
| ATOM | 385 | N   | ASN | 50 | 6.531  | 19.246 | -4.311  | 1.00 | 6.14  |
| ATOM | 386 | CA  | ASN | 50 | 5.449  | 18.729 | -3.464  | 1.00 | 5.89  |
| ATOM | 387 | CB  | ASN | 50 | 5.834  | 17.332 | -2.967  | 1.00 | 6.25  |
| ATOM | 388 | CG  | ASN | 50 | 4.688  | 16.658 | -2.270  | 1.00 | 5.80  |
| ATOM | 389 | OD1 | ASN | 50 | 3.717  | 17.297 | -1.870  | 1.00 | 7.60  |
| ATOM | 390 | ND2 | ASN | 50 | 4.840  | 15.366 | -2.058  | 1.00 | 7.26  |
| ATOM | 391 | C   | ASN | 50 | 5.184  | 19.714 | -2.331  | 1.00 | 5.68  |
| ATOM | 392 | O   | ASN | 50 | 5.744  | 19.597 | -1.230  | 1.00 | 6.62  |
| ATOM | 393 | N   | VAL | 51 | 4.328  | 20.676 | -2.619  | 1.00 | 5.97  |
| ATOM | 394 | CA  | VAL | 51 | 4.037  | 21.706 | -1.632  | 1.00 | 6.10  |
| ATOM | 395 | CB  | VAL | 51 | 3.508  | 23.010 | -2.290  | 1.00 | 6.74  |
| ATOM | 396 | CG1 | VAL | 51 | 4.557  | 23.676 | -3.184  | 1.00 | 9.06  |
| ATOM | 397 | CG2 | VAL | 51 | 2.250  | 22.743 | -3.048  | 1.00 | 9.15  |
| ATOM | 398 | C   | VAL | 51 | 3.137  | 21.232 | -0.504  | 1.00 | 7.22  |
| ATOM | 399 | O   | VAL | 51 | 3.199  | 21.758 | 0.610   | 1.00 | 7.84  |
| ATOM | 400 | N   | GLN | 52 | 2.286  | 20.231 | -0.761  | 1.00 | 7.44  |
| ATOM | 401 | CA  | GLN | 52 | 1.474  | 19.721 | 0.339   | 1.00 | 6.88  |
| ATOM | 402 | CB  | GLN | 52 | 0.442  | 18.728 | -0.163  | 1.00 | 8.70  |
| ATOM | 403 | CG  | GLN | 52 | -0.534 | 18.205 | 0.917   | 1.00 | 10.71 |
| ATOM | 404 | CD  | GLN | 52 | -0.066 | 17.059 | 1.807   | 1.00 | 12.39 |
| ATOM | 405 | OE1 | GLN | 52 | 0.970  | 16.387 | 1.579   | 1.00 | 12.25 |
| ATOM | 406 | NE2 | GLN | 52 | -0.672 | 16.925 | 2.956   | 1.00 | 13.45 |
| ATOM | 407 | C   | GLN | 52 | 2.410  | 19.094 | 1.378   | 1.00 | 6.81  |
| ATOM | 408 | O   | GLN | 52 | 2.162  | 19.264 | 2.599   | 1.00 | 6.97  |
| ATOM | 409 | N   | ARG | 53 | 3.434  | 18.364 | 0.950   | 1.00 | 6.70  |
| ATOM | 410 | CA  | ARG | 53 | 4.339  | 17.734 | 1.912   | 1.00 | 6.00  |
| ATOM | 411 | CB  | ARG | 53 | 5.152  | 16.655 | 1.210   | 1.00 | 6.55  |
| ATOM | 412 | CG  | ARG | 53 | 6.068  | 15.894 | 2.129   | 1.00 | 6.59  |
| ATOM | 413 | CD  | ARG | 53 | 6.645  | 14.676 | 1.432   | 1.00 | 8.72  |
| ATOM | 414 | NE  | ARG | 53 | 7.445  | 13.846 | 2.348   | 1.00 | 8.70  |
| ATOM | 415 | CZ  | ARG | 53 | 8.771  | 13.910 | 2.425   | 1.00 | 10.05 |
| ATOM | 416 | NH1 | ARG | 53 | 9.464  | 14.723 | 1.605   | 1.00 | 12.80 |
| ATOM | 417 | NH2 | ARG | 53 | 9.424  | 13.106 | 3.279   | 1.00 | 10.00 |
| ATOM | 418 | C   | ARG | 53 | 5.156  | 18.809 | 2.598   | 1.00 | 5.84  |
| ATOM | 419 | O   | ARG | 53 | 5.396  | 18.698 | 3.820   | 1.00 | 6.89  |
| ATOM | 420 | N   | LEU | 54 | 5.598  | 19.850 | 1.903   | 1.00 | 5.98  |
| ATOM | 421 | CA  | LEU | 54 | 6.274  | 20.982 | 2.544   | 1.00 | 5.87  |
| ATOM | 422 | CB  | LEU | 54 | 6.558  | 22.056 | 1.489   | 1.00 | 6.27  |
| ATOM | 423 | CG  | LEU | 54 | 6.940  | 23.435 | 2.017   | 1.00 | 7.00  |
| ATOM | 424 | CD1 | LEU | 54 | 8.286  | 23.396 | 2.689   | 1.00 | 7.98  |
| ATOM | 425 | CD2 | LEU | 54 | 6.864  | 24.441 | 0.866   | 1.00 | 8.66  |
| ATOM | 426 | C   | LEU | 54 | 5.406  | 21.576 | 3.660   | 1.00 | 5.97  |
| ATOM | 427 | O   | LEU | 54 | 5.870  | 21.822 | 4.788   | 1.00 | 6.89  |
| ATOM | 428 | N   | SER | 55 | 4.136  | 21.786 | 3.344   | 1.00 | 6.27  |
| ATOM | 429 | CA  | SER | 55 | 3.240  | 22.335 | 4.357   | 1.00 | 6.86  |
| ATOM | 430 | CB  | SER | 55 | 1.916  | 22.675 | 3.694   | 1.00 | 7.85  |
| ATOM | 431 | OG  | SER | 55 | 0.981  | 23.194 | 4.615   | 1.00 | 11.52 |
| ATOM | 432 | C   | SER | 55 | 3.098  | 21.410 | 5.563   | 1.00 | 6.98  |
| ATOM | 433 | O   | SER | 55 | 3.081  | 21.834 | 6.713   | 1.00 | 7.09  |
| ATOM | 434 | N   | GLN | 56 | 2.961  | 20.107 | 5.309   | 1.00 | 7.22  |

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 435 | CA  | GLN | 56 | 2.784  | 19.139 | 6.379  | 1.00 | 7.20  |
| ATOM | 436 | CB  | GLN | 56 | 2.400  | 17.795 | 5.799  | 1.00 | 9.23  |
| ATOM | 437 | CG  | GLN | 56 | 2.329  | 16.657 | 6.795  | 1.00 | 11.52 |
| ATOM | 438 | CD  | GLN | 56 | 1.214  | 16.804 | 7.803  | 1.00 | 14.79 |
| ATOM | 439 | OE1 | GLN | 56 | 1.405  | 16.302 | 8.912  | 1.00 | 22.67 |
| ATOM | 440 | NE2 | GLN | 56 | 0.122  | 17.443 | 7.423  | 1.00 | 13.58 |
| ATOM | 441 | C   | GLN | 56 | 4.007  | 19.101 | 7.279  | 1.00 | 7.77  |
| ATOM | 442 | O   | GLN | 56 | 3.869  | 19.099 | 8.517  | 1.00 | 7.98  |
| ATOM | 443 | N   | LYS | 57 | 5.188  | 18.978 | 6.684  | 1.00 | 6.97  |
| ATOM | 444 | CA  | LYS | 57 | 6.404  | 18.904 | 7.465  | 1.00 | 7.11  |
| ATOM | 445 | CB  | LYS | 57 | 7.622  | 18.583 | 6.598  | 1.00 | 7.89  |
| ATOM | 446 | CG  | LYS | 57 | 7.574  | 17.249 | 5.861  | 1.00 | 7.92  |
| ATOM | 447 | CD  | LYS | 57 | 7.561  | 16.023 | 6.784  | 1.00 | 9.42  |
| ATOM | 448 | CE  | LYS | 57 | 7.650  | 14.765 | 5.962  | 1.00 | 10.57 |
| ATOM | 449 | NZ  | LYS | 57 | 7.444  | 13.524 | 6.770  | 1.00 | 13.31 |
| ATOM | 450 | C   | LYS | 57 | 6.623  | 20.175 | 8.273  | 1.00 | 6.73  |
| ATOM | 451 | O   | LYS | 57 | 7.102  | 20.149 | 9.413  | 1.00 | 8.29  |
| ATOM | 452 | N   | THR | 58 | 6.325  | 21.322 | 7.676  | 1.00 | 7.11  |
| ATOM | 453 | CA  | THR | 58 | 6.448  | 22.618 | 8.342  | 1.00 | 7.21  |
| ATOM | 454 | CB  | THR | 58 | 6.257  | 23.767 | 7.355  | 1.00 | 7.45  |
| ATOM | 455 | OG1 | THR | 58 | 7.318  | 23.725 | 6.392  | 1.00 | 8.22  |
| ATOM | 456 | CG2 | THR | 58 | 6.316  | 25.134 | 8.054  | 1.00 | 8.05  |
| ATOM | 457 | C   | THR | 58 | 5.495  | 22.727 | 9.527  | 1.00 | 6.99  |
| ATOM | 458 | O   | THR | 58 | 5.879  | 23.194 | 10.618 | 1.00 | 7.76  |
| ATOM | 459 | N   | LYS | 59 | 4.257  | 22.255 | 9.336  | 1.00 | 7.98  |
| ATOM | 460 | CA  | LYS | 59 | 3.270  | 22.244 | 10.430 | 1.00 | 8.41  |
| ATOM | 461 | CB  | LYS | 59 | 1.933  | 21.732 | 9.870  | 1.00 | 11.31 |
| ATOM | 462 | CG  | LYS | 59 | 0.857  | 21.678 | 10.962 | 1.00 | 17.36 |
| ATOM | 463 | CD  | LYS | 59 | -0.412 | 21.032 | 10.378 | 1.00 | 21.57 |
| ATOM | 464 | CE  | LYS | 59 | -0.145 | 19.572 | 10.080 | 1.00 | 26.63 |
| ATOM | 465 | NZ  | LYS | 59 | 0.949  | 19.018 | 10.953 | 1.00 | 41.28 |
| ATOM | 466 | C   | LYS | 59 | 3.756  | 21.375 | 11.583 | 1.00 | 8.97  |
| ATOM | 467 | O   | LYS | 59 | 3.662  | 21.789 | 12.743 | 1.00 | 9.25  |
| ATOM | 468 | N   | GLU | 60 | 4.260  | 20.182 | 11.254 | 1.00 | 8.73  |
| ATOM | 469 | CA  | GLU | 60 | 4.763  | 19.297 | 12.288 | 1.00 | 9.20  |
| ATOM | 470 | CB  | GLU | 60 | 5.286  | 17.988 | 11.679 | 1.00 | 10.60 |
| ATOM | 471 | CG  | GLU | 60 | 4.189  | 17.114 | 11.083 | 1.00 | 13.69 |
| ATOM | 472 | CD  | GLU | 60 | 4.634  | 15.954 | 10.241 | 1.00 | 15.34 |
| ATOM | 473 | OE1 | GLU | 60 | 5.846  | 15.700 | 10.211 | 1.00 | 20.83 |
| ATOM | 474 | OE2 | GLU | 60 | 3.819  | 15.290 | 9.550  | 1.00 | 19.41 |
| ATOM | 475 | C   | GLU | 60 | 5.849  | 19.961 | 13.119 | 1.00 | 10.04 |
| ATOM | 476 | O   | GLU | 60 | 5.822  | 19.898 | 14.353 | 1.00 | 11.42 |
| ATOM | 477 | N   | PHE | 61 | 6.751  | 20.687 | 12.465 | 1.00 | 8.91  |
| ATOM | 478 | CA  | PHE | 61 | 7.785  | 21.443 | 13.184 | 1.00 | 7.35  |
| ATOM | 479 | CB  | PHE | 61 | 8.775  | 21.958 | 12.129 | 1.00 | 7.73  |
| ATOM | 480 | CG  | PHE | 61 | 9.763  | 22.977 | 12.665 | 1.00 | 8.40  |
| ATOM | 481 | CD1 | PHE | 61 | 10.749 | 22.594 | 13.521 | 1.00 | 9.42  |
| ATOM | 482 | CD2 | PHE | 61 | 9.667  | 24.316 | 12.302 | 1.00 | 10.73 |
| ATOM | 483 | CE1 | PHE | 61 | 11.653 | 23.520 | 13.994 | 1.00 | 10.45 |
| ATOM | 484 | CE2 | PHE | 61 | 10.591 | 25.256 | 12.727 | 1.00 | 11.37 |
| ATOM | 485 | CZ  | PHE | 61 | 11.562 | 24.834 | 13.606 | 1.00 | 10.57 |
| ATOM | 486 | C   | PHE | 61 | 7.211  | 22.579 | 14.015 | 1.00 | 7.60  |
| ATOM | 487 | O   | PHE | 61 | 7.474  | 22.658 | 15.228 | 1.00 | 8.53  |
| ATOM | 488 | N   | HIS | 62 | 6.446  | 23.487 | 13.426 | 1.00 | 8.25  |
| ATOM | 489 | CA  | HIS | 62 | 5.921  | 24.635 | 14.156 | 1.00 | 8.66  |
| ATOM | 490 | CB  | HIS | 62 | 5.076  | 25.531 | 13.261 | 1.00 | 9.03  |
| ATOM | 491 | CG  | HIS | 62 | 5.800  | 26.423 | 12.311 | 1.00 | 8.36  |
| ATOM | 492 | CD2 | HIS | 62 | 5.271  | 26.774 | 11.094 | 1.00 | 7.90  |
| ATOM | 493 | ND1 | HIS | 62 | 6.963  | 27.124 | 12.415 | 1.00 | 10.22 |
| ATOM | 494 | CE1 | HIS | 62 | 7.123  | 27.845 | 11.303 | 1.00 | 7.76  |
| ATOM | 495 | NE2 | HIS | 62 | 6.122  | 27.622 | 10.488 | 1.00 | 10.59 |
| ATOM | 496 | C   | HIS | 62 | 5.091  | 24.264 | 15.385 | 1.00 | 9.71  |
| ATOM | 497 | O   | HIS | 62 | 5.070  | 24.974 | 16.376 | 1.00 | 11.19 |
| ATOM | 498 | N   | MET | 63 | 4.335  | 23.167 | 15.283 | 1.00 | 10.41 |
| ATOM | 499 | CA  | MET | 63 | 3.393  | 22.836 | 16.321 | 1.00 | 12.27 |
| ATOM | 500 | CB  | MET | 63 | 2.151  | 22.162 | 15.705 | 1.00 | 13.32 |
| ATOM | 501 | CG  | MET | 63 | 1.453  | 23.061 | 14.692 | 1.00 | 14.13 |
| ATOM | 502 | SD  | MET | 63 | 1.062  | 24.757 | 15.253 | 1.00 | 21.44 |
| ATOM | 503 | CE  | MET | 63 | 0.528  | 25.519 | 13.715 | 1.00 | 41.15 |
| ATOM | 504 | C   | MET | 63 | 4.020  | 22.008 | 17.416 | 1.00 | 13.21 |
| ATOM | 505 | O   | MET | 63 | 3.383  | 21.818 | 18.470 | 1.00 | 19.62 |
| ATOM | 506 | N   | SER | 64 | 5.203  | 21.457 | 17.178 | 1.00 | 10.61 |
| ATOM | 507 | CA  | SER | 64 | 5.896  | 20.662 | 18.191 | 1.00 | 13.44 |

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 508 | CB  | SER | 64 | 6.289  | 19.283 | 17.662 | 1.00 | 15.70 |
| ATOM | 509 | OG  | SER | 64 | 7.299  | 19.356 | 16.689 | 1.00 | 17.37 |
| ATOM | 510 | C   | SER | 64 | 7.105  | 21.342 | 18.809 | 1.00 | 12.71 |
| ATOM | 511 | O   | SER | 64 | 7.528  | 20.933 | 19.888 | 1.00 | 16.31 |
| ATOM | 512 | N   | ILE | 65 | 7.664  | 22.392 | 18.236 | 1.00 | 10.13 |
| ATOM | 513 | CA  | ILE | 65 | 8.799  | 23.010 | 18.900 | 1.00 | 9.79  |
| ATOM | 514 | CB  | ILE | 65 | 9.469  | 23.968 | 17.906 | 1.00 | 10.92 |
| ATOM | 515 | CG2 | ILE | 65 | 8.583  | 25.072 | 17.406 | 1.00 | 13.10 |
| ATOM | 516 | CG1 | ILE | 65 | 10.787 | 24.455 | 18.502 | 1.00 | 11.85 |
| ATOM | 517 | CD1 | ILE | 65 | 11.740 | 25.156 | 17.598 | 1.00 | 13.44 |
| ATOM | 518 | C   | ILE | 65 | 8.366  | 23.703 | 20.162 | 1.00 | 10.18 |
| ATOM | 519 | O   | ILE | 65 | 7.286  | 24.267 | 20.263 | 1.00 | 12.62 |
| ATOM | 520 | N   | THR | 66 | 9.170  | 23.608 | 21.194 | 1.00 | 10.22 |
| ATOM | 521 | CA  | THR | 66 | 8.866  | 24.106 | 22.535 | 1.00 | 10.08 |
| ATOM | 522 | CB  | THR | 66 | 9.278  | 23.065 | 23.583 | 1.00 | 9.97  |
| ATOM | 523 | OG1 | THR | 66 | 10.681 | 22.892 | 23.511 | 1.00 | 12.07 |
| ATOM | 524 | CG2 | THR | 66 | 8.571  | 21.749 | 23.373 | 1.00 | 14.54 |
| ATOM | 525 | C   | THR | 66 | 9.559  | 25.420 | 22.846 | 1.00 | 8.74  |
| ATOM | 526 | O   | THR | 66 | 10.531 | 25.775 | 22.160 | 1.00 | 8.66  |
| ATOM | 527 | N   | PRO | 67 | 9.078  | 26.142 | 23.864 | 1.00 | 9.12  |
| ATOM | 528 | CD  | PRO | 67 | 7.813  | 25.938 | 24.594 | 1.00 | 11.31 |
| ATOM | 529 | CA  | PRO | 67 | 9.724  | 27.392 | 24.251 | 1.00 | 9.65  |
| ATOM | 530 | CB  | PRO | 67 | 8.925  | 27.860 | 25.450 | 1.00 | 12.19 |
| ATOM | 531 | CG  | PRO | 67 | 7.598  | 27.233 | 25.312 | 1.00 | 12.99 |
| ATOM | 532 | C   | PRO | 67 | 11.209 | 27.228 | 24.567 | 1.00 | 9.34  |
| ATOM | 533 | O   | PRO | 67 | 12.046 | 28.064 | 24.200 | 1.00 | 10.59 |
| ATOM | 534 | N   | GLU | 68 | 11.597 | 26.115 | 25.186 | 1.00 | 10.47 |
| ATOM | 535 | CA  | GLU | 68 | 13.000 | 25.861 | 25.470 | 1.00 | 11.64 |
| ATOM | 536 | CB  | GLU | 68 | 13.061 | 24.533 | 26.244 | 1.00 | 13.13 |
| ATOM | 537 | CG  | GLU | 68 | 14.452 | 24.123 | 26.600 | 1.00 | 14.22 |
| ATOM | 538 | CD  | GLU | 68 | 14.498 | 22.689 | 27.107 | 1.00 | 15.39 |
| ATOM | 539 | OE1 | GLU | 68 | 13.945 | 21.743 | 26.508 | 1.00 | 21.01 |
| ATOM | 540 | OE2 | GLU | 68 | 15.043 | 22.449 | 28.180 | 1.00 | 19.65 |
| ATOM | 541 | C   | GLU | 68 | 13.836 | 25.799 | 24.217 | 1.00 | 9.32  |
| ATOM | 542 | O   | GLU | 68 | 14.920 | 26.376 | 24.096 | 1.00 | 11.18 |
| ATOM | 543 | N   | GLU | 69 | 13.319 | 25.065 | 23.221 | 1.00 | 8.89  |
| ATOM | 544 | CA  | GLU | 69 | 14.015 | 24.920 | 21.929 | 1.00 | 9.17  |
| ATOM | 545 | CB  | GLU | 69 | 13.310 | 23.921 | 21.010 | 1.00 | 9.44  |
| ATOM | 546 | CG  | GLU | 69 | 13.338 | 22.513 | 21.576 | 1.00 | 10.83 |
| ATOM | 547 | CD  | GLU | 69 | 12.432 | 21.627 | 20.745 | 1.00 | 12.92 |
| ATOM | 548 | OE1 | GLU | 69 | 12.996 | 20.941 | 19.876 | 1.00 | 19.22 |
| ATOM | 549 | OE2 | GLU | 69 | 11.213 | 21.599 | 21.003 | 1.00 | 19.62 |
| ATOM | 550 | C   | GLU | 69 | 14.157 | 26.247 | 21.213 | 1.00 | 8.87  |
| ATOM | 551 | O   | GLU | 69 | 15.153 | 26.521 | 20.573 | 1.00 | 9.17  |
| ATOM | 552 | N   | LYS | 70 | 13.126 | 27.086 | 21.311 | 1.00 | 8.65  |
| ATOM | 553 | CA  | LYS | 70 | 13.148 | 28.387 | 20.621 | 1.00 | 8.41  |
| ATOM | 554 | CB  | LYS | 70 | 11.786 | 29.100 | 20.695 | 1.00 | 8.73  |
| ATOM | 555 | CG  | LYS | 70 | 10.663 | 28.358 | 19.977 | 1.00 | 8.40  |
| ATOM | 556 | CD  | LYS | 70 | 9.319  | 29.001 | 20.239 | 1.00 | 9.16  |
| ATOM | 557 | CE  | LYS | 70 | 8.198  | 28.102 | 19.726 | 1.00 | 10.86 |
| ATOM | 558 | NZ  | LYS | 70 | 6.875  | 28.741 | 19.900 | 1.00 | 12.00 |
| ATOM | 559 | C   | LYS | 70 | 14.268 | 29.257 | 21.182 | 1.00 | 7.77  |
| ATOM | 560 | O   | LYS | 70 | 14.992 | 29.885 | 20.400 | 1.00 | 8.10  |
| ATOM | 561 | N   | TRP | 71 | 14.418 | 29.325 | 22.514 | 1.00 | 7.55  |
| ATOM | 562 | CA  | TRP | 71 | 15.556 | 30.080 | 23.057 | 1.00 | 7.86  |
| ATOM | 563 | CB  | TRP | 71 | 15.545 | 30.104 | 24.582 | 1.00 | 8.53  |
| ATOM | 564 | CG  | TRP | 71 | 14.467 | 30.932 | 25.195 | 1.00 | 7.80  |
| ATOM | 565 | CD2 | TRP | 71 | 14.216 | 32.335 | 25.045 | 1.00 | 7.55  |
| ATOM | 566 | CE2 | TRP | 71 | 13.097 | 32.672 | 25.824 | 1.00 | 8.56  |
| ATOM | 567 | CE3 | TRP | 71 | 14.813 | 33.362 | 24.326 | 1.00 | 8.26  |
| ATOM | 568 | CD1 | TRP | 71 | 13.512 | 30.477 | 26.068 | 1.00 | 8.54  |
| ATOM | 569 | NE1 | TRP | 71 | 12.682 | 31.521 | 26.446 | 1.00 | 9.24  |
| ATOM | 570 | CZ2 | TRP | 71 | 12.589 | 33.965 | 25.900 | 1.00 | 9.23  |
| ATOM | 571 | CZ3 | TRP | 71 | 14.311 | 34.644 | 24.384 | 1.00 | 8.95  |
| ATOM | 572 | CH2 | TRP | 71 | 13.198 | 34.947 | 25.181 | 1.00 | 9.37  |
| ATOM | 573 | C   | TRP | 71 | 16.892 | 29.513 | 22.565 | 1.00 | 7.41  |
| ATOM | 574 | O   | TRP | 71 | 17.808 | 30.271 | 22.223 | 1.00 | 7.75  |
| ATOM | 575 | N   | ASP | 72 | 16.954 | 28.180 | 22.552 | 1.00 | 7.95  |
| ATOM | 576 | CA  | ASP | 72 | 18.195 | 27.508 | 22.215 | 1.00 | 9.24  |
| ATOM | 577 | CB  | ASP | 72 | 18.123 | 26.031 | 22.638 | 1.00 | 11.24 |
| ATOM | 578 | CG  | ASP | 72 | 18.208 | 25.822 | 24.146 | 1.00 | 14.08 |
| ATOM | 579 | OD1 | ASP | 72 | 18.351 | 26.778 | 24.967 | 1.00 | 15.23 |
| ATOM | 580 | OD2 | ASP | 72 | 17.942 | 24.678 | 24.599 | 1.00 | 17.93 |

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 581 | C   | ASP | 72 | 18.589 | 27.715 | 20.764 | 1.00 | 9.14  |
| ATOM | 582 | O   | ASP | 72 | 19.766 | 27.648 | 20.413 | 1.00 | 10.16 |
| ATOM | 583 | N   | LEU | 73 | 17.615 | 27.980 | 19.872 | 1.00 | 7.62  |
| ATOM | 584 | CA  | LEU | 73 | 17.828 | 28.233 | 18.474 | 1.00 | 8.24  |
| ATOM | 585 | CB  | LEU | 73 | 16.767 | 27.452 | 17.648 | 1.00 | 9.44  |
| ATOM | 586 | CG  | LEU | 73 | 16.895 | 25.941 | 17.683 | 1.00 | 10.93 |
| ATOM | 587 | CD1 | LEU | 73 | 15.676 | 25.238 | 17.093 | 1.00 | 16.41 |
| ATOM | 588 | CD2 | LEU | 73 | 18.199 | 25.437 | 17.077 | 1.00 | 14.97 |
| ATOM | 589 | C   | LEU | 73 | 17.804 | 29.708 | 18.102 | 1.00 | 7.12  |
| ATOM | 590 | O   | LEU | 73 | 17.930 | 30.074 | 16.935 | 1.00 | 7.82  |
| ATOM | 591 | N   | ALA | 74 | 17.541 | 30.607 | 19.036 | 1.00 | 6.72  |
| ATOM | 592 | CA  | ALA | 74 | 17.201 | 31.967 | 18.766 | 1.00 | 6.46  |
| ATOM | 593 | CB  | ALA | 74 | 16.742 | 32.662 | 20.042 | 1.00 | 7.96  |
| ATOM | 594 | C   | ALA | 74 | 18.258 | 32.818 | 18.098 | 1.00 | 7.50  |
| ATOM | 595 | O   | ALA | 74 | 19.423 | 32.697 | 18.490 | 1.00 | 8.38  |
| ATOM | 596 | N   | ILE | 75 | 17.864 | 33.689 | 17.172 | 1.00 | 6.76  |
| ATOM | 597 | CA  | ILE | 75 | 18.795 | 34.680 | 16.652 | 1.00 | 6.71  |
| ATOM | 598 | CB  | ILE | 75 | 18.224 | 35.376 | 15.420 | 1.00 | 6.88  |
| ATOM | 599 | CG2 | ILE | 75 | 18.044 | 34.424 | 14.239 | 1.00 | 8.21  |
| ATOM | 600 | CG1 | ILE | 75 | 16.936 | 36.140 | 15.755 | 1.00 | 7.17  |
| ATOM | 601 | CD1 | ILE | 75 | 16.522 | 37.151 | 14.715 | 1.00 | 9.71  |
| ATOM | 602 | C   | ILE | 75 | 19.201 | 35.704 | 17.734 | 1.00 | 7.09  |
| ATOM | 603 | O   | ILE | 75 | 18.546 | 35.810 | 18.781 | 1.00 | 6.89  |
| ATOM | 604 | N   | ALA | 76 | 20.280 | 36.421 | 17.461 | 1.00 | 8.25  |
| ATOM | 605 | CA  | ALA | 76 | 20.876 | 37.407 | 18.360 | 1.00 | 9.65  |
| ATOM | 606 | CB  | ALA | 76 | 22.084 | 38.067 | 17.666 | 1.00 | 16.12 |
| ATOM | 607 | C   | ALA | 76 | 19.886 | 38.445 | 18.838 | 1.00 | 8.48  |
| ATOM | 608 | O   | ALA | 76 | 19.962 | 38.940 | 19.953 | 1.00 | 9.39  |
| ATOM | 609 | N   | ALA | 77 | 18.905 | 38.810 | 18.002 | 1.00 | 8.30  |
| ATOM | 610 | CA  | ALA | 77 | 17.911 | 39.800 | 18.374 | 1.00 | 9.45  |
| ATOM | 611 | CB  | ALA | 77 | 16.992 | 40.064 | 17.179 | 1.00 | 10.84 |
| ATOM | 612 | C   | ALA | 77 | 17.100 | 39.352 | 19.582 | 1.00 | 8.44  |
| ATOM | 613 | O   | ALA | 77 | 16.541 | 40.191 | 20.299 | 1.00 | 10.71 |
| ATOM | 614 | N   | TYR | 78 | 16.967 | 38.049 | 19.816 | 1.00 | 7.56  |
| ATOM | 615 | CA  | TYR | 78 | 16.222 | 37.513 | 20.938 | 1.00 | 8.24  |
| ATOM | 616 | CB  | TYR | 78 | 15.223 | 36.420 | 20.451 | 1.00 | 7.69  |
| ATOM | 617 | CG  | TYR | 78 | 14.158 | 37.043 | 19.575 | 1.00 | 7.53  |
| ATOM | 618 | CD1 | TYR | 78 | 14.272 | 36.972 | 18.193 | 1.00 | 7.61  |
| ATOM | 619 | CE1 | TYR | 78 | 13.370 | 37.508 | 17.335 | 1.00 | 7.49  |
| ATOM | 620 | CD2 | TYR | 78 | 13.050 | 37.728 | 20.079 | 1.00 | 8.66  |
| ATOM | 621 | CE2 | TYR | 78 | 12.150 | 38.290 | 19.216 | 1.00 | 9.02  |
| ATOM | 622 | CZ  | TYR | 78 | 12.291 | 38.173 | 17.845 | 1.00 | 8.23  |
| ATOM | 623 | OH  | TYR | 78 | 11.357 | 38.805 | 17.028 | 1.00 | 10.37 |
| ATOM | 624 | C   | TYR | 78 | 17.115 | 36.920 | 22.016 | 1.00 | 7.16  |
| ATOM | 625 | O   | TYR | 78 | 16.681 | 36.716 | 23.134 | 1.00 | 10.37 |
| ATOM | 626 | N   | ASN | 79 | 18.346 | 36.542 | 21.694 | 1.00 | 8.52  |
| ATOM | 627 | CA  | ASN | 79 | 19.232 | 35.854 | 22.624 | 1.00 | 7.53  |
| ATOM | 628 | CB  | ASN | 79 | 19.164 | 34.338 | 22.379 | 1.00 | 7.59  |
| ATOM | 629 | CG  | ASN | 79 | 20.000 | 33.518 | 23.343 | 1.00 | 7.82  |
| ATOM | 630 | OD1 | ASN | 79 | 20.942 | 34.010 | 23.962 | 1.00 | 8.62  |
| ATOM | 631 | ND2 | ASN | 79 | 19.686 | 32.222 | 23.477 | 1.00 | 9.18  |
| ATOM | 632 | C   | ASN | 79 | 20.653 | 36.401 | 22.394 | 1.00 | 8.94  |
| ATOM | 633 | O   | ASN | 79 | 21.341 | 36.042 | 21.442 | 1.00 | 10.00 |
| ATOM | 634 | N   | LYS | 80 | 21.086 | 37.226 | 23.348 | 1.00 | 9.67  |
| ATOM | 635 | CA  | LYS | 80 | 22.403 | 37.853 | 23.279 | 1.00 | 11.21 |
| ATOM | 636 | CB  | LYS | 80 | 22.575 | 38.808 | 24.473 | 1.00 | 14.70 |
| ATOM | 637 | CG  | LYS | 80 | 21.697 | 40.035 | 24.385 | 1.00 | 20.93 |
| ATOM | 638 | CD  | LYS | 80 | 21.970 | 41.007 | 25.532 | 1.00 | 25.64 |
| ATOM | 639 | CE  | LYS | 80 | 21.540 | 42.420 | 25.219 | 1.00 | 29.22 |
| ATOM | 640 | NZ  | LYS | 80 | 20.209 | 42.711 | 25.795 | 1.00 | 39.86 |
| ATOM | 641 | C   | LYS | 80 | 23.565 | 36.877 | 23.274 | 1.00 | 10.80 |
| ATOM | 642 | O   | LYS | 80 | 24.702 | 37.192 | 22.944 | 1.00 | 13.45 |
| ATOM | 643 | N   | GLU | 81 | 23.349 | 35.630 | 23.706 | 1.00 | 10.06 |
| ATOM | 644 | CA  | GLU | 81 | 24.436 | 34.666 | 23.722 | 1.00 | 11.25 |
| ATOM | 645 | CB  | GLU | 81 | 24.060 | 33.385 | 24.505 | 1.00 | 11.80 |
| ATOM | 646 | CG  | GLU | 81 | 23.668 | 33.565 | 25.948 | 1.00 | 15.18 |
| ATOM | 647 | CD  | GLU | 81 | 23.394 | 32.322 | 26.768 | 1.00 | 16.40 |
| ATOM | 648 | OE1 | GLU | 81 | 22.810 | 32.379 | 27.889 | 1.00 | 16.96 |
| ATOM | 649 | OE2 | GLU | 81 | 23.688 | 31.185 | 26.315 | 1.00 | 21.03 |
| ATOM | 650 | C   | GLU | 81 | 24.791 | 34.265 | 22.281 | 1.00 | 12.20 |
| ATOM | 651 | O   | GLU | 81 | 25.838 | 33.655 | 22.069 | 1.00 | 14.12 |
| ATOM | 652 | N   | HIS | 82 | 23.900 | 34.439 | 21.316 | 1.00 | 10.21 |
| ATOM | 653 | CA  | HIS | 82 | 24.112 | 33.865 | 19.980 | 1.00 | 9.63  |

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 654 | CB  | HIS | 82 | 22.803 | 33.231 | 19.530 | 1.00 | 9.27  |
| ATOM | 655 | CG  | HIS | 82 | 22.371 | 32.070 | 20.360 | 1.00 | 9.26  |
| ATOM | 656 | CD2 | HIS | 82 | 23.068 | 31.323 | 21.257 | 1.00 | 10.67 |
| ATOM | 657 | ND1 | HIS | 82 | 21.113 | 31.516 | 20.288 | 1.00 | 8.55  |
| ATOM | 658 | CE1 | HIS | 82 | 21.063 | 30.500 | 21.141 | 1.00 | 8.43  |
| ATOM | 659 | NE2 | HIS | 82 | 22.223 | 30.366 | 21.742 | 1.00 | 10.55 |
| ATOM | 660 | C   | HIS | 82 | 24.567 | 34.933 | 19.029 | 1.00 | 10.23 |
| ATOM | 661 | O   | HIS | 82 | 23.901 | 35.266 | 18.055 | 1.00 | 11.36 |
| ATOM | 662 | N   | GLN | 83 | 25.726 | 35.507 | 19.295 | 1.00 | 12.56 |
| ATOM | 663 | CA  | GLN | 83 | 26.203 | 36.634 | 18.507 | 1.00 | 13.52 |
| ATOM | 664 | CB  | GLN | 83 | 27.470 | 37.164 | 19.181 | 1.00 | 16.22 |
| ATOM | 665 | CG  | GLN | 83 | 27.163 | 37.925 | 20.478 | 1.00 | 19.23 |
| ATOM | 666 | CD  | GLN | 83 | 26.294 | 39.148 | 20.300 | 1.00 | 20.38 |
| ATOM | 667 | OE1 | GLN | 83 | 26.558 | 40.074 | 19.536 | 1.00 | 29.81 |
| ATOM | 668 | NE2 | GLN | 83 | 25.191 | 39.208 | 21.046 | 1.00 | 22.46 |
| ATOM | 669 | C   | GLN | 83 | 26.450 | 36.332 | 17.050 | 1.00 | 13.44 |
| ATOM | 670 | O   | GLN | 83 | 26.392 | 37.262 | 16.246 | 1.00 | 15.10 |
| ATOM | 671 | N   | ASP | 84 | 26.636 | 35.089 | 16.694 | 1.00 | 13.17 |
| ATOM | 672 | CA  | ASP | 84 | 26.862 | 34.722 | 15.292 | 1.00 | 14.01 |
| ATOM | 673 | CB  | ASP | 84 | 27.692 | 33.451 | 15.162 | 1.00 | 17.37 |
| ATOM | 674 | CG  | ASP | 84 | 29.128 | 33.607 | 15.603 | 1.00 | 20.70 |
| ATOM | 675 | OD1 | ASP | 84 | 29.618 | 34.762 | 15.567 | 1.00 | 24.40 |
| ATOM | 676 | OD2 | ASP | 84 | 29.754 | 32.593 | 15.997 | 1.00 | 26.32 |
| ATOM | 677 | C   | ASP | 84 | 25.612 | 34.566 | 14.450 | 1.00 | 13.94 |
| ATOM | 678 | O   | ASP | 84 | 25.668 | 34.506 | 13.229 | 1.00 | 13.72 |
| ATOM | 679 | N   | GLN | 85 | 24.472 | 34.468 | 15.125 | 1.00 | 12.76 |
| ATOM | 680 | CA  | GLN | 85 | 23.186 | 34.270 | 14.473 | 1.00 | 11.48 |
| ATOM | 681 | CB  | GLN | 85 | 22.324 | 33.390 | 15.381 | 1.00 | 11.21 |
| ATOM | 682 | CG  | GLN | 85 | 22.791 | 31.971 | 15.552 | 1.00 | 11.91 |
| ATOM | 683 | CD  | GLN | 85 | 21.795 | 31.109 | 16.278 | 1.00 | 10.83 |
| ATOM | 684 | OE1 | GLN | 85 | 20.636 | 30.970 | 15.841 | 1.00 | 12.23 |
| ATOM | 685 | NE2 | GLN | 85 | 22.225 | 30.557 | 17.380 | 1.00 | 9.17  |
| ATOM | 686 | C   | GLN | 85 | 22.468 | 35.584 | 14.216 | 1.00 | 12.01 |
| ATOM | 687 | O   | GLN | 85 | 21.590 | 36.041 | 14.977 | 1.00 | 14.96 |
| ATOM | 688 | N   | VAL | 86 | 22.773 | 36.203 | 13.091 | 1.00 | 10.72 |
| ATOM | 689 | CA  | VAL | 86 | 22.062 | 37.392 | 12.684 | 1.00 | 11.56 |
| ATOM | 690 | CB  | VAL | 86 | 23.031 | 38.325 | 11.951 | 1.00 | 12.29 |
| ATOM | 691 | CG1 | VAL | 86 | 22.341 | 39.541 | 11.368 | 1.00 | 16.28 |
| ATOM | 692 | CG2 | VAL | 86 | 24.227 | 38.725 | 12.807 | 1.00 | 17.21 |
| ATOM | 693 | C   | VAL | 86 | 20.862 | 36.994 | 11.853 | 1.00 | 11.74 |
| ATOM | 694 | O   | VAL | 86 | 19.737 | 37.435 | 12.126 | 1.00 | 17.43 |
| ATOM | 695 | N   | ARG | 87 | 21.060 | 36.084 | 10.898 | 1.00 | 8.59  |
| ATOM | 696 | CA  | ARG | 87 | 20.044 | 35.624 | 9.972  | 1.00 | 7.72  |
| ATOM | 697 | CB  | ARG | 87 | 20.635 | 35.441 | 8.553  | 1.00 | 8.11  |
| ATOM | 698 | CG  | ARG | 87 | 21.203 | 36.706 | 7.959  | 1.00 | 8.47  |
| ATOM | 699 | CD  | ARG | 87 | 21.842 | 36.462 | 6.599  | 1.00 | 7.75  |
| ATOM | 700 | NE  | ARG | 87 | 20.829 | 36.173 | 5.609  | 1.00 | 7.39  |
| ATOM | 701 | CZ  | ARG | 87 | 21.042 | 35.691 | 4.396  | 1.00 | 6.65  |
| ATOM | 702 | NH1 | ARG | 87 | 22.260 | 35.389 | 3.959  | 1.00 | 8.68  |
| ATOM | 703 | NH2 | ARG | 87 | 20.036 | 35.471 | 3.547  | 1.00 | 7.51  |
| ATOM | 704 | C   | ARG | 87 | 19.410 | 34.289 | 10.332 | 1.00 | 7.27  |
| ATOM | 705 | O   | ARG | 87 | 18.170 | 34.129 | 10.237 | 1.00 | 8.33  |
| ATOM | 706 | N   | ALA | 88 | 20.206 | 33.270 | 10.609 | 1.00 | 7.40  |
| ATOM | 707 | CA  | ALA | 88 | 19.749 | 31.876 | 10.750 | 1.00 | 6.92  |
| ATOM | 708 | CB  | ALA | 88 | 20.760 | 30.869 | 10.254 | 1.00 | 8.59  |
| ATOM | 709 | C   | ALA | 88 | 19.373 | 31.526 | 12.165 | 1.00 | 7.06  |
| ATOM | 710 | O   | ALA | 88 | 20.138 | 31.793 | 13.084 | 1.00 | 9.57  |
| ATOM | 711 | N   | GLY | 89 | 18.191 | 30.953 | 12.332 | 1.00 | 6.44  |
| ATOM | 712 | CA  | GLY | 89 | 17.673 | 30.494 | 13.592 | 1.00 | 6.74  |
| ATOM | 713 | C   | GLY | 89 | 16.222 | 30.872 | 13.801 | 1.00 | 6.23  |
| ATOM | 714 | O   | GLY | 89 | 15.451 | 31.150 | 12.853 | 1.00 | 6.32  |
| ATOM | 715 | N   | TYR | 90 | 15.811 | 30.854 | 15.062 | 1.00 | 6.31  |
| ATOM | 716 | CA  | TYR | 90 | 14.439 | 31.063 | 15.460 | 1.00 | 6.71  |
| ATOM | 717 | CB  | TYR | 90 | 14.009 | 30.142 | 16.623 | 1.00 | 7.29  |
| ATOM | 718 | CG  | TYR | 90 | 12.552 | 29.793 | 16.487 | 1.00 | 6.81  |
| ATOM | 719 | CD1 | TYR | 90 | 12.151 | 28.687 | 15.755 | 1.00 | 7.89  |
| ATOM | 720 | CE1 | TYR | 90 | 10.830 | 28.357 | 15.592 | 1.00 | 8.96  |
| ATOM | 721 | CD2 | TYR | 90 | 11.536 | 30.556 | 17.042 | 1.00 | 7.06  |
| ATOM | 722 | CE2 | TYR | 90 | 10.193 | 30.257 | 16.837 | 1.00 | 8.48  |
| ATOM | 723 | CZ  | TYR | 90 | 9.854  | 29.145 | 16.124 | 1.00 | 9.10  |
| ATOM | 724 | OH  | TYR | 90 | 8.555  | 28.790 | 15.864 | 1.00 | 13.43 |
| ATOM | 725 | C   | TYR | 90 | 14.191 | 32.541 | 15.802 | 1.00 | 6.30  |
| ATOM | 726 | O   | TYR | 90 | 14.986 | 33.184 | 16.491 | 1.00 | 6.78  |

|      |     |     |     |     |        |        |        |      |       |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 727 | N   | TYR | 91  | 13.035 | 33.030 | 15.320 | 1.00 | 6.07  |
| ATOM | 728 | CA  | TYR | 91  | 12.554 | 34.384 | 15.484 | 1.00 | 6.47  |
| ATOM | 729 | CB  | TYR | 91  | 12.252 | 35.025 | 14.135 | 1.00 | 6.78  |
| ATOM | 730 | CG  | TYR | 91  | 13.392 | 35.277 | 13.209 | 1.00 | 6.23  |
| ATOM | 731 | CD1 | TYR | 91  | 14.353 | 34.332 | 12.859 | 1.00 | 7.06  |
| ATOM | 732 | CE1 | TYR | 91  | 15.364 | 34.597 | 11.962 | 1.00 | 7.29  |
| ATOM | 733 | CD2 | TYR | 91  | 13.490 | 36.521 | 12.556 | 1.00 | 7.46  |
| ATOM | 734 | CE2 | TYR | 91  | 14.486 | 36.776 | 11.634 | 1.00 | 7.96  |
| ATOM | 735 | CZ  | TYR | 91  | 15.428 | 35.826 | 11.343 | 1.00 | 6.61  |
| ATOM | 736 | OH  | TYR | 91  | 16.438 | 36.143 | 10.440 | 1.00 | 8.55  |
| ATOM | 737 | C   | TYR | 91  | 11.289 | 34.262 | 16.334 | 1.00 | 5.71  |
| ATOM | 738 | O   | TYR | 91  | 10.273 | 33.788 | 15.843 | 1.00 | 6.82  |
| ATOM | 739 | N   | LEU | 92  | 11.385 | 34.619 | 17.619 | 1.00 | 6.69  |
| ATOM | 740 | CA  | LEU | 92  | 10.306 | 34.337 | 18.569 | 1.00 | 6.33  |
| ATOM | 741 | CB  | LEU | 92  | 10.873 | 34.371 | 19.987 | 1.00 | 7.20  |
| ATOM | 742 | CG  | LEU | 92  | 11.700 | 33.188 | 20.466 | 1.00 | 7.89  |
| ATOM | 743 | CD1 | LEU | 92  | 13.022 | 33.065 | 19.735 | 1.00 | 10.35 |
| ATOM | 744 | CD2 | LEU | 92  | 11.888 | 33.261 | 21.985 | 1.00 | 6.37  |
| ATOM | 745 | C   | LEU | 92  | 9.151  | 35.317 | 18.471 | 1.00 | 7.36  |
| ATOM | 746 | O   | LEU | 92  | 9.284  | 36.491 | 18.161 | 1.00 | 7.12  |
| ATOM | 747 | N   | SER | 93  | 7.976  | 34.786 | 18.810 | 1.00 | 7.59  |
| ATOM | 748 | CA  | SER | 93  | 6.805  | 35.605 | 19.060 | 1.00 | 8.96  |
| ATOM | 749 | CB  | SER | 93  | 5.523  | 34.794 | 19.013 | 1.00 | 11.17 |
| ATOM | 750 | OG  | SER | 93  | 5.410  | 33.894 | 20.074 | 1.00 | 7.83  |
| ATOM | 751 | C   | SER | 93  | 6.928  | 36.224 | 20.443 | 1.00 | 8.58  |
| ATOM | 752 | O   | SER | 93  | 7.728  | 35.807 | 21.266 | 1.00 | 9.38  |
| ATOM | 753 | N   | ILE | 94  | 6.100  | 37.213 | 20.688 | 1.00 | 9.91  |
| ATOM | 754 | CA  | ILE | 94  | 6.029  | 37.865 | 22.016 | 1.00 | 10.58 |
| ATOM | 755 | CB  | ILE | 94  | 6.640  | 39.280 | 21.992 | 1.00 | 11.13 |
| ATOM | 756 | CG2 | ILE | 94  | 6.575  | 39.842 | 23.385 | 1.00 | 11.02 |
| ATOM | 757 | CG1 | ILE | 94  | 8.051  | 39.304 | 21.385 | 1.00 | 12.81 |
| ATOM | 758 | CD1 | ILE | 94  | 8.740  | 40.630 | 21.225 | 1.00 | 9.85  |
| ATOM | 759 | C   | ILE | 94  | 4.550  | 37.947 | 22.376 | 1.00 | 11.19 |
| ATOM | 760 | O   | ILE | 94  | 3.881  | 38.887 | 21.906 | 1.00 | 10.93 |
| ATOM | 761 | N   | PRO | 95  | 4.006  | 36.948 | 23.046 | 1.00 | 12.42 |
| ATOM | 762 | CD  | PRO | 95  | 4.693  | 35.749 | 23.520 | 1.00 | 12.23 |
| ATOM | 763 | CA  | PRO | 95  | 2.560  | 36.878 | 23.342 | 1.00 | 13.83 |
| ATOM | 764 | CB  | PRO | 95  | 2.394  | 35.670 | 24.234 | 1.00 | 13.55 |
| ATOM | 765 | CG  | PRO | 95  | 3.555  | 34.807 | 23.867 | 1.00 | 11.65 |
| ATOM | 766 | C   | PRO | 95  | 2.064  | 38.173 | 23.973 | 1.00 | 12.20 |
| ATOM | 767 | O   | PRO | 95  | 2.791  | 38.800 | 24.780 | 1.00 | 12.67 |
| ATOM | 768 | N   | GLY | 96  | 0.973  | 38.667 | 23.409 | 1.00 | 13.37 |
| ATOM | 769 | CA  | GLY | 96  | 0.479  | 39.965 | 23.799 | 1.00 | 12.23 |
| ATOM | 770 | C   | GLY | 96  | 0.933  | 41.142 | 22.976 | 1.00 | 15.48 |
| ATOM | 771 | O   | GLY | 96  | 0.366  | 42.233 | 23.105 | 1.00 | 12.23 |
| ATOM | 772 | N   | LYS | 97  | 1.992  | 40.975 | 22.189 | 1.00 | 11.30 |
| ATOM | 773 | CA  | LYS | 97  | 2.637  | 42.048 | 21.444 | 1.00 | 12.24 |
| ATOM | 774 | CB  | LYS | 97  | 3.947  | 42.410 | 22.187 | 1.00 | 13.52 |
| ATOM | 775 | CG  | LYS | 97  | 3.784  | 42.828 | 23.625 | 1.00 | 15.77 |
| ATOM | 776 | CD  | LYS | 97  | 3.087  | 44.147 | 23.758 | 1.00 | 18.45 |
| ATOM | 777 | CE  | LYS | 97  | 3.019  | 44.549 | 25.226 | 1.00 | 21.87 |
| ATOM | 778 | NZ  | LYS | 97  | 2.107  | 45.715 | 25.339 | 1.00 | 10.88 |
| ATOM | 779 | C   | LYS | 97  | 2.977  | 41.783 | 19.977 | 1.00 | 11.92 |
| ATOM | 780 | O   | LYS | 97  | 2.857  | 42.638 | 19.081 | 1.00 | 10.38 |
| ATOM | 781 | N   | LYS | 98  | 3.453  | 40.583 | 19.691 | 1.00 | 9.59  |
| ATOM | 782 | CA  | LYS | 98  | 3.913  | 40.149 | 18.374 | 1.00 | 12.06 |
| ATOM | 783 | CB  | LYS | 98  | 5.442  | 40.215 | 18.332 | 1.00 | 11.30 |
| ATOM | 784 | CG  | LYS | 98  | 6.093  | 39.618 | 17.105 | 1.00 | 10.99 |
| ATOM | 785 | CD  | LYS | 98  | 7.604  | 39.879 | 17.116 | 1.00 | 10.76 |
| ATOM | 786 | CE  | LYS | 98  | 8.338  | 39.370 | 15.908 | 1.00 | 10.00 |
| ATOM | 787 | NZ  | LYS | 98  | 8.448  | 37.856 | 15.937 | 1.00 | 9.52  |
| ATOM | 788 | C   | LYS | 98  | 3.462  | 38.723 | 18.145 | 1.00 | 10.44 |
| ATOM | 789 | O   | LYS | 98  | 3.835  | 37.797 | 18.884 | 1.00 | 8.69  |
| ATOM | 790 | N   | ALA | 99  | 2.674  | 38.529 | 17.108 | 1.00 | 8.30  |
| ATOM | 791 | CA  | ALA | 99  | 2.095  | 37.221 | 16.865 | 1.00 | 11.01 |
| ATOM | 792 | CB  | ALA | 99  | 0.771  | 37.440 | 16.107 | 1.00 | 7.09  |
| ATOM | 793 | C   | ALA | 99  | 2.993  | 36.289 | 16.048 | 1.00 | 8.34  |
| ATOM | 794 | O   | ALA | 99  | 3.091  | 35.086 | 16.291 | 1.00 | 7.33  |
| ATOM | 795 | N   | VAL | 100 | 3.614  | 36.851 | 14.990 | 1.00 | 7.31  |
| ATOM | 796 | CA  | VAL | 100 | 4.390  | 36.044 | 14.085 | 1.00 | 8.26  |
| ATOM | 797 | CB  | VAL | 100 | 4.804  | 36.909 | 12.882 | 1.00 | 9.84  |
| ATOM | 798 | CG1 | VAL | 100 | 5.854  | 37.965 | 13.230 | 1.00 | 9.08  |
| ATOM | 799 | CG2 | VAL | 100 | 5.294  | 36.092 | 11.703 | 1.00 |       |

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|      |     |     |     |     |        |        |        |      |       |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 800 | C   | VAL | 100 | 5.636  | 35.463 | 14.759 | 1.00 | 6.77  |
| ATOM | 801 | O   | VAL | 100 | 6.274  | 36.069 | 15.614 | 1.00 | 6.24  |
| ATOM | 802 | N   | GLU | 101 | 6.039  | 34.294 | 14.261 | 1.00 | 5.93  |
| ATOM | 803 | CA  | GLU | 101 | 7.275  | 33.647 | 14.643 | 1.00 | 5.89  |
| ATOM | 804 | CB  | GLU | 101 | 7.164  | 32.758 | 15.864 | 1.00 | 6.83  |
| ATOM | 805 | CG  | GLU | 101 | 6.194  | 31.599 | 15.714 | 1.00 | 9.01  |
| ATOM | 806 | CD  | GLU | 101 | 5.993  | 30.900 | 17.058 | 1.00 | 11.15 |
| ATOM | 807 | OE1 | GLU | 101 | 4.957  | 31.171 | 17.727 | 1.00 | 11.35 |
| ATOM | 808 | OE2 | GLU | 101 | 6.839  | 30.033 | 17.396 | 1.00 | 16.56 |
| ATOM | 809 | C   | GLU | 101 | 7.748  | 32.835 | 13.441 | 1.00 | 6.12  |
| ATOM | 810 | O   | GLU | 101 | 6.989  | 32.513 | 12.532 | 1.00 | 6.44  |
| ATOM | 811 | N   | SER | 102 | 9.047  | 32.564 | 13.384 | 1.00 | 6.02  |
| ATOM | 812 | CA  | SER | 102 | 9.605  | 31.897 | 12.196 | 1.00 | 6.00  |
| ATOM | 813 | CB  | SER | 102 | 9.725  | 32.906 | 11.058 | 1.00 | 6.77  |
| ATOM | 814 | OG  | SER | 102 | 10.632 | 33.935 | 11.388 | 1.00 | 7.64  |
| ATOM | 815 | C   | SER | 102 | 10.934 | 31.253 | 12.468 | 1.00 | 6.15  |
| ATOM | 816 | O   | SER | 102 | 11.592 | 31.497 | 13.474 | 1.00 | 6.61  |
| ATOM | 817 | N   | PHE | 103 | 11.367 | 30.433 | 11.517 | 1.00 | 5.73  |
| ATOM | 818 | CA  | PHE | 103 | 12.670 | 29.792 | 11.506 | 1.00 | 5.88  |
| ATOM | 819 | CB  | PHE | 103 | 12.521 | 28.294 | 11.756 | 1.00 | 6.37  |
| ATOM | 820 | CG  | PHE | 103 | 13.795 | 27.476 | 11.663 | 1.00 | 6.21  |
| ATOM | 821 | CD1 | PHE | 103 | 14.723 | 27.499 | 12.686 | 1.00 | 7.53  |
| ATOM | 822 | CD2 | PHE | 103 | 14.034 | 26.650 | 10.562 | 1.00 | 7.03  |
| ATOM | 823 | CE1 | PHE | 103 | 15.866 | 26.713 | 12.620 | 1.00 | 7.78  |
| ATOM | 824 | CE2 | PHE | 103 | 15.167 | 25.887 | 10.483 | 1.00 | 6.93  |
| ATOM | 825 | CZ  | PHE | 103 | 16.077 | 25.924 | 11.508 | 1.00 | 7.07  |
| ATOM | 826 | C   | PHE | 103 | 13.319 | 30.018 | 10.149 | 1.00 | 5.84  |
| ATOM | 827 | O   | PHE | 103 | 12.720 | 29.679 | 9.124  | 1.00 | 5.89  |
| ATOM | 828 | N   | CYS | 104 | 14.505 | 30.596 | 10.128 | 1.00 | 5.38  |
| ATOM | 829 | CA  | CYS | 104 | 15.244 | 30.888 | 8.907  | 1.00 | 5.34  |
| ATOM | 830 | CB  | CYS | 104 | 15.669 | 32.368 | 8.935  | 1.00 | 6.38  |
| ATOM | 831 | SG  | CYS | 104 | 16.693 | 32.902 | 7.544  | 1.00 | 7.14  |
| ATOM | 832 | C   | CYS | 104 | 16.475 | 29.988 | 8.802  | 1.00 | 5.05  |
| ATOM | 833 | O   | CYS | 104 | 17.202 | 29.801 | 9.794  | 1.00 | 5.55  |
| ATOM | 834 | N   | TYR | 105 | 16.758 | 29.512 | 7.615  | 1.00 | 5.01  |
| ATOM | 835 | CA  | TYR | 105 | 17.979 | 28.794 | 7.344  | 1.00 | 4.98  |
| ATOM | 836 | CB  | TYR | 105 | 17.839 | 27.285 | 7.499  | 1.00 | 5.67  |
| ATOM | 837 | CG  | TYR | 105 | 16.822 | 26.594 | 6.589  | 1.00 | 5.07  |
| ATOM | 838 | CD1 | TYR | 105 | 17.258 | 25.856 | 5.491  | 1.00 | 5.34  |
| ATOM | 839 | CE1 | TYR | 105 | 16.371 | 25.171 | 4.659  | 1.00 | 5.87  |
| ATOM | 840 | CD2 | TYR | 105 | 15.469 | 26.551 | 6.883  | 1.00 | 5.19  |
| ATOM | 841 | CE2 | TYR | 105 | 14.595 | 25.862 | 6.059  | 1.00 | 5.89  |
| ATOM | 842 | CZ  | TYR | 105 | 15.045 | 25.169 | 4.966  | 1.00 | 5.38  |
| ATOM | 843 | OH  | TYR | 105 | 14.141 | 24.495 | 4.169  | 1.00 | 6.39  |
| ATOM | 844 | C   | TYR | 105 | 18.515 | 29.202 | 5.972  | 1.00 | 4.38  |
| ATOM | 845 | O   | TYR | 105 | 17.778 | 29.622 | 5.072  | 1.00 | 5.26  |
| ATOM | 846 | N   | LEU | 106 | 19.816 | 29.039 | 5.852  | 1.00 | 5.00  |
| ATOM | 847 | CA  | LEU | 106 | 20.634 | 29.415 | 4.731  | 1.00 | 4.93  |
| ATOM | 848 | CB  | LEU | 106 | 21.803 | 30.266 | 5.227  | 1.00 | 6.26  |
| ATOM | 849 | CG  | LEU | 106 | 21.444 | 31.467 | 6.125  | 1.00 | 6.45  |
| ATOM | 850 | CD1 | LEU | 106 | 22.709 | 32.219 | 6.477  | 1.00 | 8.37  |
| ATOM | 851 | CD2 | LEU | 106 | 20.392 | 32.329 | 5.466  | 1.00 | 6.90  |
| ATOM | 852 | C   | LEU | 106 | 21.121 | 28.188 | 3.948  | 1.00 | 4.77  |
| ATOM | 853 | O   | LEU | 106 | 20.754 | 27.046 | 4.237  | 1.00 | 5.93  |
| ATOM | 854 | N   | ASN | 107 | 21.991 | 28.473 | 2.983  | 1.00 | 4.96  |
| ATOM | 855 | CA  | ASN | 107 | 22.654 | 27.437 | 2.187  | 1.00 | 5.23  |
| ATOM | 856 | CB  | ASN | 107 | 23.803 | 28.147 | 1.434  | 1.00 | 5.83  |
| ATOM | 857 | CG  | ASN | 107 | 24.424 | 27.280 | 0.353  | 1.00 | 5.32  |
| ATOM | 858 | OD1 | ASN | 107 | 24.420 | 26.044 | 0.396  | 1.00 | 5.91  |
| ATOM | 859 | ND2 | ASN | 107 | 24.989 | 27.988 | -0.626 | 1.00 | 6.49  |
| ATOM | 860 | C   | ASN | 107 | 23.225 | 26.347 | 3.079  | 1.00 | 4.82  |
| ATOM | 861 | O   | ASN | 107 | 24.097 | 26.593 | 3.937  | 1.00 | 5.62  |
| ATOM | 862 | N   | PRO | 108 | 22.771 | 25.095 | 2.881  | 1.00 | 4.96  |
| ATOM | 863 | CD  | PRO | 108 | 21.595 | 24.677 | 2.118  | 1.00 | 5.43  |
| ATOM | 864 | CA  | PRO | 108 | 23.345 | 23.973 | 3.639  | 1.00 | 5.82  |
| ATOM | 865 | CB  | PRO | 108 | 22.516 | 22.773 | 3.134  | 1.00 | 6.84  |
| ATOM | 866 | CG  | PRO | 108 | 21.194 | 23.377 | 2.749  | 1.00 | 6.32  |
| ATOM | 867 | C   | PRO | 108 | 24.846 | 23.763 | 3.444  | 1.00 | 5.93  |
| ATOM | 868 | O   | PRO | 108 | 25.533 | 23.129 | 4.274  | 1.00 | 6.51  |
| ATOM | 869 | N   | ASN | 109 | 25.397 | 24.277 | 2.353  | 1.00 | 5.53  |
| ATOM | 870 | CA  | ASN | 109 | 26.823 | 24.180 | 2.080  | 1.00 | 5.84  |
| ATOM | 871 | CB  | ASN | 109 | 27.130 | 24.369 | 0.598  | 1.00 | 6.10  |
| ATOM | 872 | CG  | ASN | 109 | 26.633 | 23.186 | -0.200 | 1.00 | 5.51  |

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|      |     |     |     |     |        |        |        |      |       |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 873 | OD1 | ASN | 109 | 26.690 | 22.020 | 0.209  | 1.00 | 7.43  |
| ATOM | 874 | ND2 | ASN | 109 | 26.165 | 23.491 | -1.405 | 1.00 | 7.14  |
| ATOM | 875 | C   | ASN | 109 | 27.652 | 25.150 | 2.920  | 1.00 | 5.95  |
| ATOM | 876 | O   | ASN | 109 | 28.863 | 25.063 | 2.911  | 1.00 | 6.60  |
| ATOM | 877 | N   | PHE | 110 | 27.032 | 26.060 | 3.672  | 1.00 | 6.52  |
| ATOM | 878 | CA  | PHE | 110 | 27.727 | 26.943 | 4.602  | 1.00 | 6.64  |
| ATOM | 879 | CB  | PHE | 110 | 26.984 | 28.235 | 4.934  | 1.00 | 6.86  |
| ATOM | 880 | CG  | PHE | 110 | 26.793 | 29.203 | 3.781  | 1.00 | 6.62  |
| ATOM | 881 | CD1 | PHE | 110 | 27.454 | 29.100 | 2.593  | 1.00 | 6.42  |
| ATOM | 882 | CD2 | PHE | 110 | 25.889 | 30.238 | 3.919  | 1.00 | 7.13  |
| ATOM | 883 | CE1 | PHE | 110 | 27.269 | 30.020 | 1.570  | 1.00 | 7.97  |
| ATOM | 884 | CE2 | PHE | 110 | 25.698 | 31.178 | 2.917  | 1.00 | 7.73  |
| ATOM | 885 | CZ  | PHE | 110 | 26.380 | 31.064 | 1.723  | 1.00 | 7.68  |
| ATOM | 886 | C   | PHE | 110 | 28.010 | 26.131 | 5.870  | 1.00 | 6.41  |
| ATOM | 887 | O   | PHE | 110 | 27.334 | 26.222 | 6.890  | 1.00 | 9.08  |
| ATOM | 888 | N   | THR | 111 | 29.047 | 25.319 | 5.795  | 1.00 | 7.20  |
| ATOM | 889 | CA  | THR | 111 | 29.543 | 24.473 | 6.858  | 1.00 | 7.97  |
| ATOM | 890 | CB  | THR | 111 | 29.986 | 23.114 | 6.240  | 1.00 | 9.61  |
| ATOM | 891 | OG1 | THR | 111 | 30.863 | 23.407 | 5.150  | 1.00 | 12.08 |
| ATOM | 892 | CG2 | THR | 111 | 28.831 | 22.332 | 5.660  | 1.00 | 11.21 |
| ATOM | 893 | C   | THR | 111 | 30.719 | 25.173 | 7.535  | 1.00 | 8.55  |
| ATOM | 894 | O   | THR | 111 | 31.262 | 26.161 | 7.039  | 1.00 | 8.43  |
| ATOM | 895 | N   | PRO | 112 | 31.158 | 24.669 | 8.690  | 1.00 | 10.82 |
| ATOM | 896 | CD  | PRO | 112 | 30.500 | 23.646 | 9.514  | 1.00 | 12.34 |
| ATOM | 897 | CA  | PRO | 112 | 32.284 | 25.317 | 9.365  | 1.00 | 10.76 |
| ATOM | 898 | CB  | PRO | 112 | 32.454 | 24.403 | 10.591 | 1.00 | 12.53 |
| ATOM | 899 | CG  | PRO | 112 | 31.035 | 23.971 | 10.884 | 1.00 | 13.67 |
| ATOM | 900 | C   | PRO | 112 | 33.560 | 25.453 | 8.553  | 1.00 | 10.13 |
| ATOM | 901 | O   | PRO | 112 | 34.293 | 26.449 | 8.719  | 1.00 | 12.02 |
| ATOM | 902 | N   | ASP | 113 | 33.764 | 24.577 | 7.586  | 1.00 | 10.28 |
| ATOM | 903 | CA  | ASP | 113 | 34.960 | 24.594 | 6.754  | 1.00 | 11.85 |
| ATOM | 904 | CB  | ASP | 113 | 35.418 | 23.179 | 6.354  | 1.00 | 14.15 |
| ATOM | 905 | CG  | ASP | 113 | 34.450 | 22.335 | 5.556  | 1.00 | 16.88 |
| ATOM | 906 | OD1 | ASP | 113 | 34.697 | 21.122 | 5.265  | 1.00 | 17.94 |
| ATOM | 907 | OD2 | ASP | 113 | 33.431 | 22.903 | 5.120  | 1.00 | 18.33 |
| ATOM | 908 | C   | ASP | 113 | 34.779 | 25.485 | 5.516  | 1.00 | 10.04 |
| ATOM | 909 | O   | ASP | 113 | 35.695 | 25.568 | 4.674  | 1.00 | 11.29 |
| ATOM | 910 | N   | HIS | 114 | 33.614 | 26.058 | 5.256  | 1.00 | 8.19  |
| ATOM | 911 | CA  | HIS | 114 | 33.388 | 26.853 | 4.066  | 1.00 | 7.72  |
| ATOM | 912 | CB  | HIS | 114 | 31.924 | 27.234 | 3.945  | 1.00 | 8.19  |
| ATOM | 913 | CG  | HIS | 114 | 31.514 | 27.896 | 2.661  | 1.00 | 7.35  |
| ATOM | 914 | CD2 | HIS | 114 | 30.786 | 27.365 | 1.634  | 1.00 | 7.63  |
| ATOM | 915 | ND1 | HIS | 114 | 31.853 | 29.194 | 2.350  | 1.00 | 7.74  |
| ATOM | 916 | CE1 | HIS | 114 | 31.374 | 29.423 | 1.125  | 1.00 | 8.63  |
| ATOM | 917 | NE2 | HIS | 114 | 30.698 | 28.385 | 0.701  | 1.00 | 8.22  |
| ATOM | 918 | C   | HIS | 114 | 34.263 | 28.078 | 4.069  | 1.00 | 7.89  |
| ATOM | 919 | O   | HIS | 114 | 34.363 | 28.705 | 5.126  | 1.00 | 8.23  |
| ATOM | 920 | N   | PRO | 115 | 34.877 | 28.447 | 2.947  | 1.00 | 8.07  |
| ATOM | 921 | CD  | PRO | 115 | 34.805 | 27.853 | 1.595  | 1.00 | 9.44  |
| ATOM | 922 | CA  | PRO | 115 | 35.791 | 29.586 | 2.989  | 1.00 | 7.97  |
| ATOM | 923 | CB  | PRO | 115 | 36.432 | 29.638 | 1.603  | 1.00 | 10.29 |
| ATOM | 924 | CG  | PRO | 115 | 36.058 | 28.363 | 0.935  | 1.00 | 16.51 |
| ATOM | 925 | C   | PRO | 115 | 35.213 | 30.906 | 3.451  | 1.00 | 8.16  |
| ATOM | 926 | O   | PRO | 115 | 35.957 | 31.749 | 4.033  | 1.00 | 8.89  |
| ATOM | 927 | N   | ARG | 116 | 33.935 | 31.156 | 3.245  | 1.00 | 7.57  |
| ATOM | 928 | CA  | ARG | 116 | 33.282 | 32.366 | 3.687  | 1.00 | 8.05  |
| ATOM | 929 | CB  | ARG | 116 | 32.055 | 32.649 | 2.831  | 1.00 | 9.75  |
| ATOM | 930 | CG  | ARG | 116 | 32.363 | 33.041 | 1.398  | 1.00 | 11.43 |
| ATOM | 931 | CD  | ARG | 116 | 33.024 | 34.444 | 1.316  | 1.00 | 17.12 |
| ATOM | 932 | NE  | ARG | 116 | 32.909 | 34.976 | -0.046 | 1.00 | 18.64 |
| ATOM | 933 | CZ  | ARG | 116 | 33.267 | 36.202 | -0.332 | 1.00 | 16.55 |
| ATOM | 934 | NH1 | ARG | 116 | 33.732 | 37.005 | 0.626  | 1.00 | 18.90 |
| ATOM | 935 | NH2 | ARG | 116 | 33.158 | 36.628 | -1.550 | 1.00 | 19.38 |
| ATOM | 936 | C   | ARG | 116 | 32.955 | 32.353 | 5.168  | 1.00 | 8.18  |
| ATOM | 937 | O   | ARG | 116 | 32.905 | 33.426 | 5.807  | 1.00 | 10.55 |
| ATOM | 938 | N   | ILE | 117 | 32.701 | 31.161 | 5.702  | 1.00 | 7.91  |
| ATOM | 939 | CA  | ILE | 117 | 32.507 | 30.993 | 7.134  | 1.00 | 8.74  |
| ATOM | 940 | CB  | ILE | 117 | 31.884 | 29.617 | 7.425  | 1.00 | 8.27  |
| ATOM | 941 | CG2 | ILE | 117 | 31.909 | 29.337 | 8.920  | 1.00 | 10.79 |
| ATOM | 942 | CG1 | ILE | 117 | 30.482 | 29.510 | 6.798  | 1.00 | 7.78  |
| ATOM | 943 | CD1 | ILE | 117 | 29.478 | 30.458 | 7.376  | 1.00 | 9.72  |
| ATOM | 944 | C   | ILE | 117 | 33.863 | 31.170 | 7.818  | 1.00 | 9.52  |
| ATOM | 945 | O   | ILE | 117 | 33.956 | 31.893 | 8.820  | 1.00 | 10.02 |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 946  | N   | GLN | 118 | 34.936 | 30.601 | 7.248  | 1.00 | 9.60  |
| ATOM | 947  | CA  | GLN | 118 | 36.264 | 30.823 | 7.814  | 1.00 | 9.55  |
| ATOM | 948  | CB  | GLN | 118 | 37.287 | 29.975 | 7.066  | 1.00 | 11.20 |
| ATOM | 949  | CG  | GLN | 118 | 37.163 | 28.475 | 7.285  | 1.00 | 11.87 |
| ATOM | 950  | CD  | GLN | 118 | 37.706 | 28.064 | 8.628  | 1.00 | 15.84 |
| ATOM | 951  | OE1 | GLN | 118 | 38.799 | 28.509 | 9.021  | 1.00 | 16.95 |
| ATOM | 952  | NE2 | GLN | 118 | 36.968 | 27.189 | 9.314  | 1.00 | 18.58 |
| ATOM | 953  | C   | GLN | 118 | 36.524 | 32.301 | 7.782  | 1.00 | 10.34 |
| ATOM | 954  | O   | GLN | 118 | 37.209 | 32.780 | 8.779  | 1.00 | 12.18 |
| ATOM | 955  | N   | ALA | 119 | 36.307 | 33.008 | 6.719  | 1.00 | 10.58 |
| ATOM | 956  | CA  | ALA | 119 | 36.652 | 34.437 | 6.577  | 1.00 | 11.17 |
| ATOM | 957  | CB  | ALA | 119 | 36.675 | 34.884 | 5.141  | 1.00 | 11.90 |
| ATOM | 958  | C   | ALA | 119 | 35.766 | 35.340 | 7.417  | 1.00 | 11.81 |
| ATOM | 959  | O   | ALA | 119 | 35.975 | 36.547 | 7.593  | 1.00 | 13.51 |
| ATOM | 960  | N   | LYS | 120 | 34.677 | 34.792 | 7.926  | 1.00 | 11.51 |
| ATOM | 961  | CA  | LYS | 120 | 33.697 | 35.524 | 8.728  | 1.00 | 11.83 |
| ATOM | 962  | CB  | LYS | 120 | 34.314 | 36.156 | 9.981  | 1.00 | 16.43 |
| ATOM | 963  | CG  | LYS | 120 | 35.156 | 35.192 | 10.773 | 1.00 | 20.21 |
| ATOM | 964  | CD  | LYS | 120 | 34.452 | 34.007 | 11.336 | 1.00 | 25.82 |
| ATOM | 965  | CE  | LYS | 120 | 35.422 | 33.080 | 12.083 | 1.00 | 26.48 |
| ATOM | 966  | NZ  | LYS | 120 | 36.364 | 32.304 | 11.194 | 1.00 | 23.67 |
| ATOM | 967  | C   | LYS | 120 | 33.033 | 36.623 | 7.910  | 1.00 | 12.07 |
| ATOM | 968  | O   | LYS | 120 | 32.701 | 37.698 | 8.413  | 1.00 | 13.32 |
| ATOM | 969  | N   | THR | 121 | 32.773 | 36.290 | 6.647  | 1.00 | 11.59 |
| ATOM | 970  | CA  | THR | 121 | 32.162 | 37.294 | 5.783  | 1.00 | 11.41 |
| ATOM | 971  | CB  | THR | 121 | 32.158 | 36.758 | 4.336  | 1.00 | 11.74 |
| ATOM | 972  | OG1 | THR | 121 | 33.515 | 36.460 | 3.947  | 1.00 | 14.18 |
| ATOM | 973  | CG2 | THR | 121 | 31.617 | 37.825 | 3.394  | 1.00 | 13.26 |
| ATOM | 974  | C   | THR | 121 | 30.742 | 37.599 | 6.199  | 1.00 | 10.30 |
| ATOM | 975  | O   | THR | 121 | 30.016 | 36.627 | 6.442  | 1.00 | 9.38  |
| ATOM | 976  | N   | PRO | 122 | 30.343 | 38.869 | 6.255  | 1.00 | 11.24 |
| ATOM | 977  | CD  | PRO | 122 | 31.175 | 40.087 | 6.162  | 1.00 | 13.40 |
| ATOM | 978  | CA  | PRO | 122 | 28.938 | 39.176 | 6.605  | 1.00 | 10.67 |
| ATOM | 979  | CB  | PRO | 122 | 28.883 | 40.676 | 6.374  | 1.00 | 13.30 |
| ATOM | 980  | CG  | PRO | 122 | 30.251 | 41.155 | 6.684  | 1.00 | 14.04 |
| ATOM | 981  | C   | PRO | 122 | 27.933 | 38.454 | 5.721  | 1.00 | 8.90  |
| ATOM | 982  | O   | PRO | 122 | 28.224 | 38.174 | 4.567  | 1.00 | 9.02  |
| ATOM | 983  | N   | THR | 123 | 26.810 | 38.105 | 6.329  | 1.00 | 9.47  |
| ATOM | 984  | CA  | THR | 123 | 25.660 | 37.447 | 5.729  | 1.00 | 8.42  |
| ATOM | 985  | CB  | THR | 123 | 25.112 | 38.105 | 4.455  | 1.00 | 9.93  |
| ATOM | 986  | OG1 | THR | 123 | 25.929 | 37.810 | 3.314  | 1.00 | 10.18 |
| ATOM | 987  | CG2 | THR | 123 | 25.024 | 39.629 | 4.512  | 1.00 | 13.04 |
| ATOM | 988  | C   | THR | 123 | 25.807 | 35.938 | 5.560  | 1.00 | 8.70  |
| ATOM | 989  | O   | THR | 123 | 24.815 | 35.273 | 5.198  | 1.00 | 9.15  |
| ATOM | 990  | N   | HIS | 124 | 26.994 | 35.395 | 5.833  | 1.00 | 8.34  |
| ATOM | 991  | CA  | HIS | 124 | 27.189 | 33.957 | 5.798  | 1.00 | 7.64  |
| ATOM | 992  | CB  | HIS | 124 | 28.524 | 33.584 | 5.149  | 1.00 | 7.45  |
| ATOM | 993  | CG  | HIS | 124 | 28.726 | 34.113 | 3.780  | 1.00 | 7.00  |
| ATOM | 994  | CD2 | HIS | 124 | 28.755 | 33.507 | 2.577  | 1.00 | 7.26  |
| ATOM | 995  | ND1 | HIS | 124 | 28.998 | 35.449 | 3.557  | 1.00 | 7.88  |
| ATOM | 996  | CE1 | HIS | 124 | 29.202 | 35.607 | 2.261  | 1.00 | 8.29  |
| ATOM | 997  | NE2 | HIS | 124 | 29.032 | 34.478 | 1.631  | 1.00 | 7.93  |
| ATOM | 998  | C   | HIS | 124 | 27.170 | 33.387 | 7.206  | 1.00 | 8.19  |
| ATOM | 999  | O   | HIS | 124 | 27.888 | 33.913 | 8.056  | 1.00 | 9.00  |
| ATOM | 1000 | N   | GLU | 125 | 26.413 | 32.313 | 7.455  | 1.00 | 7.36  |
| ATOM | 1001 | CA  | GLU | 125 | 26.337 | 31.694 | 8.776  | 1.00 | 7.74  |
| ATOM | 1002 | CB  | GLU | 125 | 25.166 | 32.230 | 9.604  | 1.00 | 8.77  |
| ATOM | 1003 | CG  | GLU | 125 | 25.164 | 33.714 | 9.832  | 1.00 | 9.78  |
| ATOM | 1004 | CD  | GLU | 125 | 23.885 | 34.235 | 10.445 | 1.00 | 9.41  |
| ATOM | 1005 | OE1 | GLU | 125 | 23.057 | 33.439 | 10.972 | 1.00 | 12.02 |
| ATOM | 1006 | OE2 | GLU | 125 | 23.791 | 35.476 | 10.373 | 1.00 | 12.25 |
| ATOM | 1007 | C   | GLU | 125 | 26.118 | 30.196 | 8.567  | 1.00 | 7.57  |
| ATOM | 1008 | O   | GLU | 125 | 25.581 | 29.787 | 7.521  | 1.00 | 8.65  |
| ATOM | 1009 | N   | VAL | 126 | 26.505 | 29.398 | 9.557  | 1.00 | 7.88  |
| ATOM | 1010 | CA  | VAL | 126 | 26.219 | 27.969 | 9.636  | 1.00 | 7.38  |
| ATOM | 1011 | CB  | VAL | 126 | 27.281 | 27.246 | 10.488 | 1.00 | 8.22  |
| ATOM | 1012 | CG1 | VAL | 126 | 26.979 | 25.754 | 10.561 | 1.00 | 9.54  |
| ATOM | 1013 | CG2 | VAL | 126 | 28.686 | 27.497 | 9.941  | 1.00 | 9.36  |
| ATOM | 1014 | C   | VAL | 126 | 24.843 | 27.785 | 10.272 | 1.00 | 7.39  |
| ATOM | 1015 | O   | VAL | 126 | 24.564 | 28.311 | 11.344 | 1.00 | 8.29  |
| ATOM | 1016 | N   | ASN | 127 | 23.951 | 27.081 | 9.554  | 1.00 | 6.96  |
| ATOM | 1017 | CA  | ASN | 127 | 22.618 | 26.839 | 10.081 | 1.00 | 6.87  |
| ATOM | 1018 | CB  | ASN | 127 | 21.832 | 25.948 | 9.120  | 1.00 | 6.56  |

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1019 | CG  | ASN | 127 | 21.515 | 26.650 | 7.803  | 1.00 | 6.11  |
| ATOM | 1020 | OD1 | ASN | 127 | 21.362 | 27.877 | 7.793  | 1.00 | 7.19  |
| ATOM | 1021 | ND2 | ASN | 127 | 21.350 | 25.859 | 6.758  | 1.00 | 7.23  |
| ATOM | 1022 | C   | ASN | 127 | 22.624 | 26.173 | 11.447 | 1.00 | 7.20  |
| ATOM | 1023 | O   | ASN | 127 | 23.503 | 25.353 | 11.763 | 1.00 | 8.68  |
| ATOM | 1024 | N   | VAL | 128 | 21.596 | 26.511 | 12.239 | 1.00 | 7.13  |
| ATOM | 1025 | CA  | VAL | 128 | 21.284 | 25.849 | 13.501 | 1.00 | 7.06  |
| ATOM | 1026 | CB  | VAL | 128 | 21.172 | 26.848 | 14.657 | 1.00 | 8.77  |
| ATOM | 1027 | CG1 | VAL | 128 | 22.508 | 27.567 | 14.825 | 1.00 | 10.68 |
| ATOM | 1028 | CG2 | VAL | 128 | 19.986 | 27.774 | 14.501 | 1.00 | 9.46  |
| ATOM | 1029 | C   | VAL | 128 | 20.032 | 25.032 | 13.329 | 1.00 | 6.59  |
| ATOM | 1030 | O   | VAL | 128 | 19.101 | 25.426 | 12.617 | 1.00 | 8.06  |
| ATOM | 1031 | N   | TRP | 129 | 19.977 | 23.861 | 13.963 | 1.00 | 7.79  |
| ATOM | 1032 | CA  | TRP | 129 | 18.884 | 22.914 | 13.812 | 1.00 | 7.98  |
| ATOM | 1033 | CB  | TRP | 129 | 19.316 | 21.709 | 12.955 | 1.00 | 7.99  |
| ATOM | 1034 | CG  | TRP | 129 | 19.671 | 22.145 | 11.553 | 1.00 | 7.47  |
| ATOM | 1035 | CD2 | TRP | 129 | 18.743 | 22.448 | 10.496 | 1.00 | 6.77  |
| ATOM | 1036 | CE2 | TRP | 129 | 19.486 | 22.838 | 9.368  | 1.00 | 6.74  |
| ATOM | 1037 | CE3 | TRP | 129 | 17.353 | 22.428 | 10.400 | 1.00 | 6.42  |
| ATOM | 1038 | CD1 | TRP | 129 | 20.887 | 22.349 | 11.033 | 1.00 | 8.81  |
| ATOM | 1039 | NE1 | TRP | 129 | 20.809 | 22.765 | 9.721  | 1.00 | 8.43  |
| ATOM | 1040 | CZ2 | TRP | 129 | 18.902 | 23.196 | 8.160  | 1.00 | 6.63  |
| ATOM | 1041 | CZ3 | TRP | 129 | 16.754 | 22.796 | 9.207  | 1.00 | 7.42  |
| ATOM | 1042 | CH2 | TRP | 129 | 17.553 | 23.187 | 8.120  | 1.00 | 6.84  |
| ATOM | 1043 | C   | TRP | 129 | 18.434 | 22.394 | 15.187 | 1.00 | 8.10  |
| ATOM | 1044 | O   | TRP | 129 | 19.266 | 22.268 | 16.108 | 1.00 | 9.20  |
| ATOM | 1045 | N   | PRO | 130 | 17.158 | 22.038 | 15.321 | 1.00 | 11.04 |
| ATOM | 1046 | CD  | PRO | 130 | 16.078 | 22.208 | 14.338 | 1.00 | 10.04 |
| ATOM | 1047 | CA  | PRO | 130 | 16.684 | 21.410 | 16.563 | 1.00 | 12.74 |
| ATOM | 1048 | CB  | PRO | 130 | 15.190 | 21.366 | 16.377 | 1.00 | 12.90 |
| ATOM | 1049 | CG  | PRO | 130 | 14.987 | 21.348 | 14.930 | 1.00 | 10.76 |
| ATOM | 1050 | C   | PRO | 130 | 17.295 | 20.019 | 16.674 | 1.00 | 10.41 |
| ATOM | 1051 | O   | PRO | 130 | 17.902 | 19.473 | 15.742 | 1.00 | 12.19 |
| ATOM | 1052 | N   | ASP | 131 | 17.139 | 19.412 | 17.840 | 1.00 | 13.83 |
| ATOM | 1053 | CA  | ASP | 131 | 17.611 | 18.063 | 18.062 | 1.00 | 20.75 |
| ATOM | 1054 | CB  | ASP | 131 | 17.311 | 17.695 | 19.499 | 1.00 | 30.05 |
| ATOM | 1055 | CG  | ASP | 131 | 18.290 | 18.307 | 20.474 | 1.00 | 41.54 |
| ATOM | 1056 | OD1 | ASP | 131 | 19.218 | 19.075 | 20.122 | 1.00 | 44.79 |
| ATOM | 1057 | OD2 | ASP | 131 | 18.111 | 17.974 | 21.678 | 1.00 | 12.28 |
| ATOM | 1058 | C   | ASP | 131 | 16.864 | 17.077 | 17.175 | 1.00 | 11.37 |
| ATOM | 1059 | O   | ASP | 131 | 15.643 | 17.091 | 17.104 | 1.00 | 11.37 |
| ATOM | 1060 | N   | GLU | 132 | 17.632 | 16.204 | 16.561 | 1.00 | 12.37 |
| ATOM | 1061 | CA  | GLU | 132 | 17.032 | 15.236 | 15.660 | 1.00 | 14.40 |
| ATOM | 1062 | CB  | GLU | 132 | 18.140 | 14.416 | 14.986 | 1.00 | 14.02 |
| ATOM | 1063 | CG  | GLU | 132 | 17.667 | 13.221 | 14.169 | 1.00 | 14.20 |
| ATOM | 1064 | CD  | GLU | 132 | 17.004 | 13.617 | 12.890 | 1.00 | 13.96 |
| ATOM | 1065 | OE1 | GLU | 132 | 17.327 | 14.733 | 12.391 | 1.00 | 14.71 |
| ATOM | 1066 | OE2 | GLU | 132 | 16.222 | 12.787 | 12.395 | 1.00 | 13.05 |
| ATOM | 1067 | C   | GLU | 132 | 16.028 | 14.309 | 16.327 | 1.00 | 13.21 |
| ATOM | 1068 | O   | GLU | 132 | 15.022 | 13.953 | 15.730 | 1.00 | 15.02 |
| ATOM | 1069 | N   | THR | 133 | 16.283 | 13.922 | 17.576 | 1.00 | 17.13 |
| ATOM | 1070 | CA  | THR | 133 | 15.337 | 13.065 | 18.267 | 1.00 | 19.10 |
| ATOM | 1071 | CB  | THR | 133 | 15.911 | 12.663 | 19.645 | 1.00 | 30.56 |
| ATOM | 1072 | OG1 | THR | 133 | 16.214 | 13.817 | 20.436 | 1.00 | 21.80 |
| ATOM | 1073 | CG2 | THR | 133 | 17.200 | 11.914 | 19.407 | 1.00 | 14.81 |
| ATOM | 1074 | C   | THR | 133 | 14.003 | 13.738 | 18.504 | 1.00 | 18.31 |
| ATOM | 1075 | O   | THR | 133 | 12.976 | 13.052 | 18.539 | 1.00 | 14.08 |
| ATOM | 1076 | N   | LYS | 134 | 13.992 | 15.065 | 18.681 | 1.00 | 14.05 |
| ATOM | 1077 | CA  | LYS | 134 | 12.738 | 15.763 | 18.943 | 1.00 | 16.10 |
| ATOM | 1078 | CB  | LYS | 134 | 13.028 | 17.072 | 19.683 | 1.00 | 21.50 |
| ATOM | 1079 | CG  | LYS | 134 | 13.566 | 16.783 | 21.105 | 1.00 | 24.72 |
| ATOM | 1080 | CD  | LYS | 134 | 13.739 | 18.052 | 21.912 | 1.00 | 29.07 |
| ATOM | 1081 | CE  | LYS | 134 | 13.962 | 17.851 | 23.411 | 1.00 | 35.66 |
| ATOM | 1082 | NZ  | LYS | 134 | 15.380 | 17.498 | 23.673 | 1.00 | 11.72 |
| ATOM | 1083 | C   | LYS | 134 | 11.982 | 16.084 | 17.673 | 1.00 | 12.75 |
| ATOM | 1084 | O   | LYS | 134 | 10.764 | 16.268 | 17.697 | 1.00 | 10.34 |
| ATOM | 1085 | N   | HIS | 135 | 12.768 | 16.210 | 16.602 | 1.00 | 9.70  |
| ATOM | 1086 | CA  | HIS | 135 | 12.229 | 16.559 | 15.278 | 1.00 | 10.46 |
| ATOM | 1087 | CB  | HIS | 135 | 12.568 | 18.014 | 14.927 | 1.00 | 11.60 |
| ATOM | 1088 | CG  | HIS | 135 | 11.859 | 18.971 | 15.855 | 1.00 | 11.74 |
| ATOM | 1089 | CD2 | HIS | 135 | 10.625 | 19.519 | 15.664 | 1.00 | 13.42 |
| ATOM | 1090 | ND1 | HIS | 135 | 12.334 | 19.405 | 17.077 | 1.00 | 10.37 |
| ATOM | 1091 | CE1 | HIS | 135 | 11.390 | 20.219 | 17.592 | 1.00 |       |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1092 | NE2 | HIS | 135 | 10.358 | 20.261 | 16.753 | 1.00 | 14.68 |
| ATOM | 1093 | C   | HIS | 135 | 12.753 | 15.614 | 14.207 | 1.00 | 9.49  |
| ATOM | 1094 | O   | HIS | 135 | 13.491 | 16.005 | 13.302 | 1.00 | 8.95  |
| ATOM | 1095 | N   | PRO | 136 | 12.410 | 14.336 | 14.298 | 1.00 | 10.29 |
| ATOM | 1096 | CD  | PRO | 136 | 11.539 | 13.714 | 15.288 | 1.00 | 12.71 |
| ATOM | 1097 | CA  | PRO | 136 | 12.996 | 13.348 | 13.367 | 1.00 | 10.63 |
| ATOM | 1098 | CB  | PRO | 136 | 12.331 | 12.025 | 13.738 | 1.00 | 13.20 |
| ATOM | 1099 | CG  | PRO | 136 | 11.373 | 12.308 | 14.821 | 1.00 | 15.42 |
| ATOM | 1100 | C   | PRO | 136 | 12.727 | 13.656 | 11.902 | 1.00 | 9.37  |
| ATOM | 1101 | O   | PRO | 136 | 11.583 | 13.947 | 11.540 | 1.00 | 10.11 |
| ATOM | 1102 | N   | GLY | 137 | 13.801 | 13.643 | 11.131 | 1.00 | 9.15  |
| ATOM | 1103 | CA  | GLY | 137 | 13.642 | 13.906 | 9.700  | 1.00 | 8.92  |
| ATOM | 1104 | C   | GLY | 137 | 13.568 | 15.351 | 9.281  | 1.00 | 8.41  |
| ATOM | 1105 | O   | GLY | 137 | 13.604 | 15.660 | 8.076  | 1.00 | 8.62  |
| ATOM | 1106 | N   | PHE | 138 | 13.438 | 16.290 | 10.230 | 1.00 | 7.77  |
| ATOM | 1107 | CA  | PHE | 138 | 13.189 | 17.683 | 9.858  | 1.00 | 7.53  |
| ATOM | 1108 | CB  | PHE | 138 | 12.791 | 18.533 | 11.069 | 1.00 | 9.20  |
| ATOM | 1109 | CG  | PHE | 138 | 12.676 | 20.014 | 10.773 | 1.00 | 8.61  |
| ATOM | 1110 | CD1 | PHE | 138 | 11.623 | 20.502 | 9.999  | 1.00 | 8.98  |
| ATOM | 1111 | CD2 | PHE | 138 | 13.628 | 20.897 | 11.264 | 1.00 | 8.98  |
| ATOM | 1112 | CE1 | PHE | 138 | 11.598 | 21.878 | 9.728  | 1.00 | 9.14  |
| ATOM | 1113 | CE2 | PHE | 138 | 13.584 | 22.238 | 11.007 | 1.00 | 9.39  |
| ATOM | 1114 | CZ  | PHE | 138 | 12.555 | 22.730 | 10.231 | 1.00 | 8.60  |
| ATOM | 1115 | C   | PHE | 138 | 14.355 | 18.318 | 9.123  | 1.00 | 6.57  |
| ATOM | 1116 | O   | PHE | 138 | 14.155 | 18.953 | 8.090  | 1.00 | 6.31  |
| ATOM | 1117 | N   | GLN | 139 | 15.553 | 18.234 | 9.700  | 1.00 | 7.35  |
| ATOM | 1118 | CA  | GLN | 139 | 16.718 | 18.827 | 9.045  | 1.00 | 7.49  |
| ATOM | 1119 | CB  | GLN | 139 | 17.990 | 18.600 | 9.867  | 1.00 | 7.76  |
| ATOM | 1120 | CG  | GLN | 139 | 19.211 | 19.123 | 9.164  | 1.00 | 8.03  |
| ATOM | 1121 | CD  | GLN | 139 | 20.475 | 19.034 | 10.008 | 1.00 | 9.61  |
| ATOM | 1122 | OE1 | GLN | 139 | 20.452 | 18.629 | 11.194 | 1.00 | 11.81 |
| ATOM | 1123 | NE2 | GLN | 139 | 21.556 | 19.403 | 9.361  | 1.00 | 10.42 |
| ATOM | 1124 | C   | GLN | 139 | 16.898 | 18.263 | 7.634  | 1.00 | 6.36  |
| ATOM | 1125 | O   | GLN | 139 | 17.148 | 19.042 | 6.703  | 1.00 | 6.70  |
| ATOM | 1126 | N   | ASP | 140 | 16.792 | 16.962 | 7.476  | 1.00 | 7.41  |
| ATOM | 1127 | CA  | ASP | 140 | 16.966 | 16.359 | 6.153  | 1.00 | 8.02  |
| ATOM | 1128 | CB  | ASP | 140 | 17.014 | 14.845 | 6.267  | 1.00 | 10.06 |
| ATOM | 1129 | CG  | ASP | 140 | 18.185 | 14.414 | 7.143  | 1.00 | 12.56 |
| ATOM | 1130 | OD1 | ASP | 140 | 19.263 | 15.008 | 7.017  | 1.00 | 15.40 |
| ATOM | 1131 | OD2 | ASP | 140 | 18.010 | 13.419 | 7.863  | 1.00 | 17.99 |
| ATOM | 1132 | C   | ASP | 140 | 15.903 | 16.836 | 5.173  | 1.00 | 7.03  |
| ATOM | 1133 | O   | ASP | 140 | 16.195 | 17.125 | 4.012  | 1.00 | 7.37  |
| ATOM | 1134 | N   | PHE | 141 | 14.649 | 16.886 | 5.632  | 1.00 | 6.76  |
| ATOM | 1135 | CA  | PHE | 141 | 13.592 | 17.404 | 4.806  | 1.00 | 6.92  |
| ATOM | 1136 | CB  | PHE | 141 | 12.241 | 17.315 | 5.525  | 1.00 | 8.28  |
| ATOM | 1137 | CG  | PHE | 141 | 11.180 | 18.059 | 4.700  | 1.00 | 10.59 |
| ATOM | 1138 | CD1 | PHE | 141 | 10.649 | 17.398 | 3.585  | 1.00 | 12.85 |
| ATOM | 1139 | CD2 | PHE | 141 | 10.766 | 19.326 | 4.979  | 1.00 | 12.09 |
| ATOM | 1140 | CE1 | PHE | 141 | 9.773  | 18.045 | 2.730  | 1.00 | 14.79 |
| ATOM | 1141 | CE2 | PHE | 141 | 9.946  | 20.027 | 4.097  | 1.00 | 12.80 |
| ATOM | 1142 | CZ  | PHE | 141 | 9.514  | 19.385 | 2.960  | 1.00 | 15.56 |
| ATOM | 1143 | C   | PHE | 141 | 13.898 | 18.843 | 4.381  | 1.00 | 6.10  |
| ATOM | 1144 | O   | PHE | 141 | 13.715 | 19.227 | 3.224  | 1.00 | 5.52  |
| ATOM | 1145 | N   | ALA | 142 | 14.235 | 19.692 | 5.355  | 1.00 | 5.91  |
| ATOM | 1146 | CA  | ALA | 142 | 14.436 | 21.113 | 5.109  | 1.00 | 6.07  |
| ATOM | 1147 | CB  | ALA | 142 | 14.597 | 21.835 | 6.444  | 1.00 | 6.15  |
| ATOM | 1148 | C   | ALA | 142 | 15.593 | 21.396 | 4.153  | 1.00 | 5.38  |
| ATOM | 1149 | O   | ALA | 142 | 15.534 | 22.273 | 3.289  | 1.00 | 5.69  |
| ATOM | 1150 | N   | GLU | 143 | 16.660 | 20.630 | 4.306  | 1.00 | 5.79  |
| ATOM | 1151 | CA  | GLU | 143 | 17.811 | 20.759 | 3.404  | 1.00 | 5.89  |
| ATOM | 1152 | CB  | GLU | 143 | 19.021 | 19.977 | 3.912  | 1.00 | 6.66  |
| ATOM | 1153 | CG  | GLU | 143 | 19.647 | 20.589 | 5.171  | 1.00 | 6.49  |
| ATOM | 1154 | CD  | GLU | 143 | 20.818 | 19.857 | 5.742  | 1.00 | 8.57  |
| ATOM | 1155 | OE1 | GLU | 143 | 20.986 | 18.661 | 5.468  | 1.00 | 15.50 |
| ATOM | 1156 | OE2 | GLU | 143 | 21.529 | 20.401 | 6.607  | 1.00 | 8.03  |
| ATOM | 1157 | C   | GLU | 143 | 17.426 | 20.335 | 1.982  | 1.00 | 6.15  |
| ATOM | 1158 | O   | GLU | 143 | 17.798 | 21.030 | 1.046  | 1.00 | 6.03  |
| ATOM | 1159 | N   | GLN | 144 | 16.717 | 19.195 | 1.852  | 1.00 | 6.24  |
| ATOM | 1160 | CA  | GLN | 144 | 16.249 | 18.793 | 0.519  | 1.00 | 5.81  |
| ATOM | 1161 | CB  | GLN | 144 | 15.582 | 17.418 | 0.622  | 1.00 | 7.33  |
| ATOM | 1162 | CG  | GLN | 144 | 15.034 | 16.900 | -0.718 | 1.00 | 9.38  |
| ATOM | 1163 | CD  | GLN | 144 | 16.102 | 16.723 | -1.755 | 1.00 | 11.31 |
| ATOM | 1164 | OE1 | GLN | 144 | 16.165 | 17.336 | -2.852 | 1.00 | 15.13 |

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 1165 | NE2 | GLN | 144 | 17.017 | 15.794 | -1.443  | 1.00 | 13.37 |
| ATOM | 1166 | C   | GLN | 144 | 15.322 | 19.843 | -0.068  | 1.00 | 6.08  |
| ATOM | 1167 | O   | GLN | 144 | 15.367 | 20.113 | -1.286  | 1.00 | 6.65  |
| ATOM | 1168 | N   | TYR | 145 | 14.450 | 20.464 | 0.723   | 1.00 | 5.44  |
| ATOM | 1169 | CA  | TYR | 145 | 13.552 | 21.492 | 0.249   | 1.00 | 5.36  |
| ATOM | 1170 | CB  | TYR | 145 | 12.562 | 21.956 | 1.318   | 1.00 | 5.45  |
| ATOM | 1171 | CG  | TYR | 145 | 11.718 | 23.094 | 0.785   | 1.00 | 5.34  |
| ATOM | 1172 | CD1 | TYR | 145 | 10.850 | 22.844 | -0.266  | 1.00 | 5.77  |
| ATOM | 1173 | CE1 | TYR | 145 | 10.113 | 23.856 | -0.832  | 1.00 | 5.40  |
| ATOM | 1174 | CD2 | TYR | 145 | 11.863 | 24.392 | 1.209   | 1.00 | 6.05  |
| ATOM | 1175 | CE2 | TYR | 145 | 11.128 | 25.428 | 0.632   | 1.00 | 5.52  |
| ATOM | 1176 | CZ  | TYR | 145 | 10.260 | 25.146 | -0.376  | 1.00 | 4.90  |
| ATOM | 1177 | OH  | TYR | 145 | 9.505  | 26.126 | -1.002  | 1.00 | 6.57  |
| ATOM | 1178 | C   | TYR | 145 | 14.350 | 22.668 | -0.324  | 1.00 | 4.85  |
| ATOM | 1179 | O   | TYR | 145 | 14.009 | 23.173 | -1.384  | 1.00 | 5.67  |
| ATOM | 1180 | N   | TYR | 146 | 15.400 | 23.055 | 0.370   | 1.00 | 5.22  |
| ATOM | 1181 | CA  | TYR | 146 | 16.294 | 24.134 | -0.108  | 1.00 | 5.07  |
| ATOM | 1182 | CB  | TYR | 146 | 17.492 | 24.302 | 0.818   | 1.00 | 6.31  |
| ATOM | 1183 | CG  | TYR | 146 | 18.356 | 25.533 | 0.554   | 1.00 | 5.63  |
| ATOM | 1184 | CD1 | TYR | 146 | 18.217 | 26.654 | 1.367   | 1.00 | 4.93  |
| ATOM | 1185 | CE1 | TYR | 146 | 19.975 | 27.804 | 1.191   | 1.00 | 4.66  |
| ATOM | 1186 | CD2 | TYR | 146 | 19.292 | 25.595 | -0.471  | 1.00 | 5.91  |
| ATOM | 1187 | CE2 | TYR | 146 | 20.050 | 26.728 | -0.673  | 1.00 | 5.60  |
| ATOM | 1188 | CZ  | TYR | 146 | 19.892 | 27.816 | 0.151   | 1.00 | 5.33  |
| ATOM | 1189 | OH  | TYR | 146 | 20.681 | 28.929 | -0.076  | 1.00 | 6.01  |
| ATOM | 1190 | C   | TYR | 146 | 16.740 | 23.831 | -1.547  | 1.00 | 4.88  |
| ATOM | 1191 | O   | TYR | 146 | 16.630 | 24.691 | -2.413  | 1.00 | 5.89  |
| ATOM | 1192 | N   | TRP | 147 | 17.186 | 22.580 | -1.792  | 1.00 | 5.20  |
| ATOM | 1193 | CA  | TRP | 147 | 17.650 | 22.244 | -3.129  | 1.00 | 5.95  |
| ATOM | 1194 | CB  | TRP | 147 | 18.544 | 20.995 | -3.105  | 1.00 | 6.61  |
| ATOM | 1195 | CG  | TRP | 147 | 19.730 | 21.259 | -2.221  | 1.00 | 6.71  |
| ATOM | 1196 | CD2 | TRP | 147 | 20.675 | 22.345 | -2.390  | 1.00 | 6.87  |
| ATOM | 1197 | CE2 | TRP | 147 | 21.598 | 22.227 | -1.334  | 1.00 | 7.71  |
| ATOM | 1198 | CE3 | TRP | 147 | 20.828 | 23.398 | -3.303  | 1.00 | 7.63  |
| ATOM | 1199 | CD1 | TRP | 147 | 20.127 | 20.576 | -1.120  | 1.00 | 7.42  |
| ATOM | 1200 | NE1 | TRP | 147 | 21.230 | 21.118 | -0.574  | 1.00 | 7.49  |
| ATOM | 1201 | CZ2 | TRP | 147 | 22.641 | 23.133 | -1.198  | 1.00 | 8.32  |
| ATOM | 1202 | CZ3 | TRP | 147 | 21.873 | 24.299 | -3.147  | 1.00 | 8.76  |
| ATOM | 1203 | CH2 | TRP | 147 | 22.774 | 24.162 | 2.079   | 1.00 | 8.40  |
| ATOM | 1204 | C   | TRP | 147 | 16.514 | 22.124 | -4.123  | 1.00 | 5.56  |
| ATOM | 1205 | O   | TRP | 147 | 16.697 | 22.484 | -5.295  | 1.00 | 6.90  |
| ATOM | 1206 | N   | ASP | 148 | 15.333 | 21.663 | -3.736  | 1.00 | 5.62  |
| ATOM | 1207 | CA  | ASP | 148 | 14.192 | 21.610 | -4.644  | 1.00 | 6.73  |
| ATOM | 1208 | CB  | ASP | 148 | 13.006 | 20.892 | -3.990  | 1.00 | 7.41  |
| ATOM | 1209 | CG  | ASP | 148 | 13.180 | 19.397 | -3.794  | 1.00 | 9.94  |
| ATOM | 1210 | OD1 | ASP | 148 | 14.107 | 18.824 | -4.385  | 1.00 | 11.03 |
| ATOM | 1211 | OD2 | ASP | 148 | 12.308 | 18.805 | -3.115  | 1.00 | 12.94 |
| ATOM | 1212 | C   | ASP | 148 | 13.602 | 23.288 | -5.076  | 1.00 | 6.41  |
| ATOM | 1213 | O   | ASP | 148 | 13.807 | 23.013 | -6.281  | 1.00 | 6.39  |
| ATOM | 1214 | N   | VAL | 149 | 13.678 | 23.959 | -4.112  | 1.00 | 5.67  |
| ATOM | 1215 | CA  | VAL | 149 | 13.287 | 25.330 | -4.472  | 1.00 | 5.45  |
| ATOM | 1216 | CB  | VAL | 149 | 12.664 | 26.047 | -3.279  | 1.00 | 5.40  |
| ATOM | 1217 | CG1 | VAL | 149 | 13.656 | 26.460 | -2.202  | 1.00 | 5.95  |
| ATOM | 1218 | CG2 | VAL | 149 | 11.883 | 27.265 | -3.771  | 1.00 | 6.77  |
| ATOM | 1219 | C   | VAL | 149 | 14.421 | 26.084 | -5.158  | 1.00 | 5.36  |
| ATOM | 1220 | O   | VAL | 149 | 14.173 | 26.951 | -6.016  | 1.00 | 5.85  |
| ATOM | 1221 | N   | PHE | 150 | 15.669 | 25.750 | -4.879  | 1.00 | 5.71  |
| ATOM | 1222 | CA  | PHE | 150 | 16.795 | 26.267 | -5.635  | 1.00 | 5.05  |
| ATOM | 1223 | CB  | PHE | 150 | 18.111 | 25.675 | -5.056  | 1.00 | 6.21  |
| ATOM | 1224 | CG  | PHE | 150 | 19.374 | 26.154 | -5.764  | 1.00 | 6.04  |
| ATOM | 1225 | CD1 | PHE | 150 | 20.158 | 27.164 | -5.267  | 1.00 | 7.32  |
| ATOM | 1226 | CD2 | PHE | 150 | 19.840 | 25.565 | -6.911  | 1.00 | 7.41  |
| ATOM | 1227 | CE1 | PHE | 150 | 21.279 | 27.602 | -5.932  | 1.00 | 7.77  |
| ATOM | 1228 | CE2 | PHE | 150 | 20.926 | 26.005 | -7.649  | 1.00 | 8.49  |
| ATOM | 1229 | CZ  | PHE | 150 | 21.686 | 27.017 | -7.119  | 1.00 | 7.48  |
| ATOM | 1230 | C   | PHE | 150 | 16.616 | 25.887 | -7.102  | 1.00 | 5.89  |
| ATOM | 1231 | O   | PHE | 150 | 16.841 | 26.726 | -8.004  | 1.00 | 6.52  |
| ATOM | 1232 | N   | GLY | 151 | 16.276 | 24.637 | -7.351  | 1.00 | 6.70  |
| ATOM | 1233 | CA  | GLY | 151 | 16.124 | 24.168 | -8.744  | 1.00 | 6.74  |
| ATOM | 1234 | C   | GLY | 151 | 15.012 | 24.887 | -9.476  | 1.00 | 6.45  |
| ATOM | 1235 | O   | GLY | 151 | 15.150 | 25.293 | -10.619 | 1.00 | 7.27  |
| ATOM | 1236 | N   | LEU | 152 | 13.867 | 25.094 | -8.825  | 1.00 | 6.82  |
| ATOM | 1237 | CA  | LEU | 152 | 12.787 | 25.878 | -9.404  | 1.00 | 6.24  |

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 1238 | CB  | LEU | 152 | 11.582 | 25.881 | -8.452  | 1.00 | 6.29  |
| ATOM | 1239 | CG  | LEU | 152 | 10.452 | 26.859 | -8.828  | 1.00 | 7.25  |
| ATOM | 1240 | CD1 | LEU | 152 | 9.864  | 26.532 | -10.214 | 1.00 | 9.19  |
| ATOM | 1241 | CD2 | LEU | 152 | 9.358  | 26.832 | -7.763  | 1.00 | 7.05  |
| ATOM | 1242 | C   | LEU | 152 | 13.269 | 27.298 | -9.669  | 1.00 | 6.42  |
| ATOM | 1243 | O   | LEU | 152 | 13.015 | 27.864 | -10.743 | 1.00 | 7.31  |
| ATOM | 1244 | N   | SER | 153 | 13.998 | 27.874 | -8.702  | 1.00 | 5.98  |
| ATOM | 1245 | CA  | SER | 153 | 14.442 | 29.262 | -8.845  | 1.00 | 6.16  |
| ATOM | 1246 | CB  | SER | 153 | 15.068 | 29.742 | -7.541  | 1.00 | 6.44  |
| ATOM | 1247 | OG  | SER | 153 | 14.090 | 29.755 | -6.522  | 1.00 | 6.18  |
| ATOM | 1248 | C   | SER | 153 | 15.424 | 29.413 | -10.000 | 1.00 | 6.14  |
| ATOM | 1249 | O   | SER | 153 | 15.368 | 30.420 | -10.740 | 1.00 | 6.53  |
| ATOM | 1250 | N   | SER | 154 | 16.284 | 28.436 | -10.217 | 1.00 | 6.45  |
| ATOM | 1251 | CA  | SER | 154 | 17.220 | 28.495 | -11.340 | 1.00 | 7.39  |
| ATOM | 1252 | CB  | SER | 154 | 18.126 | 27.271 | -11.278 | 1.00 | 8.84  |
| ATOM | 1253 | OG  | SER | 154 | 18.981 | 27.292 | 10.189  | 1.00 | 13.14 |
| ATOM | 1254 | C   | SER | 154 | 16.418 | 28.472 | -12.643 | 1.00 | 7.57  |
| ATOM | 1255 | O   | SER | 154 | 16.742 | 29.253 | -13.563 | 1.00 | 8.31  |
| ATOM | 1256 | N   | ALA | 155 | 15.408 | 27.630 | -12.737 | 1.00 | 6.91  |
| ATOM | 1257 | CA  | ALA | 155 | 14.550 | 27.622 | -13.938 | 1.00 | 7.39  |
| ATOM | 1258 | CB  | ALA | 155 | 13.530 | 26.520 | -13.807 | 1.00 | 7.77  |
| ATOM | 1259 | C   | ALA | 155 | 13.878 | 28.964 | -14.140 | 1.00 | 6.87  |
| ATOM | 1260 | O   | ALA | 155 | 13.895 | 29.538 | -15.242 | 1.00 | 7.86  |
| ATOM | 1261 | N   | LEU | 156 | 13.323 | 29.547 | -13.083 | 1.00 | 6.99  |
| ATOM | 1262 | CA  | LEU | 156 | 12.656 | 30.860 | -13.176 | 1.00 | 5.86  |
| ATOM | 1263 | CB  | LEU | 156 | 12.035 | 31.279 | -11.838 | 1.00 | 5.92  |
| ATOM | 1264 | CG  | LEU | 156 | 10.864 | 30.434 | -11.365 | 1.00 | 5.99  |
| ATOM | 1265 | CD1 | LEU | 156 | 10.480 | 30.809 | -9.936  | 1.00 | 8.87  |
| ATOM | 1266 | CD2 | LEU | 156 | 9.686  | 30.596 | -12.284 | 1.00 | 11.48 |
| ATOM | 1267 | C   | LEU | 156 | 13.640 | 31.933 | -13.642 | 1.00 | 6.11  |
| ATOM | 1268 | O   | LEU | 156 | 13.287 | 32.805 | -14.447 | 1.00 | 7.28  |
| ATOM | 1269 | N   | LEU | 157 | 14.884 | 31.880 | -13.141 | 1.00 | 6.74  |
| ATOM | 1270 | CA  | LEU | 157 | 15.898 | 32.863 | -13.543 | 1.00 | 7.25  |
| ATOM | 1271 | CB  | LEU | 157 | 17.152 | 32.739 | -12.694 | 1.00 | 6.79  |
| ATOM | 1272 | CG  | LEU | 157 | 17.073 | 33.236 | -11.250 | 1.00 | 7.78  |
| ATOM | 1273 | CD1 | LEU | 157 | 18.408 | 33.026 | -10.580 | 1.00 | 8.46  |
| ATOM | 1274 | CD2 | LEU | 157 | 16.631 | 34.672 | -11.145 | 1.00 | 9.12  |
| ATOM | 1275 | C   | LEU | 157 | 16.227 | 32.748 | -15.028 | 1.00 | 6.91  |
| ATOM | 1276 | O   | LEU | 157 | 16.580 | 33.763 | -15.638 | 1.00 | 7.24  |
| ATOM | 1277 | N   | LYS | 158 | 16.142 | 31.561 | -15.606 | 1.00 | 7.38  |
| ATOM | 1278 | CA  | LYS | 158 | 16.335 | 31.410 | -17.057 | 1.00 | 7.07  |
| ATOM | 1279 | CB  | LYS | 158 | 16.381 | 29.927 | -17.407 | 1.00 | 9.01  |
| ATOM | 1280 | CG  | LYS | 158 | 17.574 | 29.170 | -16.887 | 1.00 | 10.48 |
| ATOM | 1281 | CD  | LYS | 158 | 17.541 | 27.683 | -17.122 | 1.00 | 13.42 |
| ATOM | 1282 | CE  | LYS | 158 | 18.743 | 27.039 | -16.407 | 1.00 | 18.16 |
| ATOM | 1283 | NZ  | LYS | 158 | 18.743 | 25.572 | -16.586 | 1.00 | 18.72 |
| ATOM | 1284 | C   | LYS | 158 | 15.185 | 32.121 | -17.782 | 1.00 | 7.00  |
| ATOM | 1285 | O   | LYS | 158 | 15.447 | 32.806 | -18.770 | 1.00 | 9.09  |
| ATOM | 1286 | N   | GLY | 159 | 13.951 | 32.032 | -17.281 | 1.00 | 7.17  |
| ATOM | 1287 | CA  | GLY | 159 | 12.834 | 32.752 | -17.873 | 1.00 | 7.22  |
| ATOM | 1288 | C   | GLY | 159 | 13.038 | 34.252 | -17.763 | 1.00 | 6.90  |
| ATOM | 1289 | O   | GLY | 159 | 12.756 | 34.973 | -18.731 | 1.00 | 7.59  |
| ATOM | 1290 | N   | TYR | 160 | 13.443 | 34.771 | -16.620 | 1.00 | 7.51  |
| ATOM | 1291 | CA  | TYR | 160 | 13.674 | 36.230 | -16.489 | 1.00 | 6.84  |
| ATOM | 1292 | CB  | TYR | 160 | 14.004 | 36.595 | -15.059 | 1.00 | 7.03  |
| ATOM | 1293 | CG  | TYR | 160 | 12.831 | 36.759 | -14.120 | 1.00 | 6.77  |
| ATOM | 1294 | CD1 | TYR | 160 | 12.421 | 35.752 | -13.251 | 1.00 | 6.69  |
| ATOM | 1295 | CE1 | TYR | 160 | 11.353 | 35.915 | -12.430 | 1.00 | 7.61  |
| ATOM | 1296 | CD2 | TYR | 160 | 12.097 | 37.948 | -14.093 | 1.00 | 7.26  |
| ATOM | 1297 | CE2 | TYR | 160 | 11.013 | 38.108 | -13.247 | 1.00 | 7.77  |
| ATOM | 1298 | CZ  | TYR | 160 | 10.643 | 37.083 | -12.380 | 1.00 | 7.26  |
| ATOM | 1299 | OH  | TYR | 160 | 9.594  | 37.202 | -11.495 | 1.00 | 8.86  |
| ATOM | 1300 | C   | TYR | 160 | 14.756 | 36.704 | -17.446 | 1.00 | 6.38  |
| ATOM | 1301 | O   | TYR | 160 | 14.653 | 37.777 | -18.003 | 1.00 | 7.25  |
| ATOM | 1302 | N   | ALA | 161 | 15.849 | 35.968 | -17.537 | 1.00 | 7.30  |
| ATOM | 1303 | CA  | ALA | 161 | 16.929 | 36.375 | -18.438 | 1.00 | 7.63  |
| ATOM | 1304 | CB  | ALA | 161 | 18.083 | 35.387 | -18.293 | 1.00 | 9.13  |
| ATOM | 1305 | C   | ALA | 161 | 16.414 | 36.456 | -19.886 | 1.00 | 7.60  |
| ATOM | 1306 | O   | ALA | 161 | 16.688 | 37.458 | -20.577 | 1.00 | 8.23  |
| ATOM | 1307 | N   | LEU | 162 | 15.755 | 35.401 | -20.331 | 1.00 | 7.75  |
| ATOM | 1308 | CA  | LEU | 162 | 15.234 | 35.423 | -21.721 | 1.00 | 7.67  |
| ATOM | 1309 | CB  | LEU | 162 | 14.537 | 34.094 | -22.022 | 1.00 | 7.94  |
| ATOM | 1310 | CG  | LEU | 162 | 15.447 | 32.872 | -22.168 | 1.00 | 8.36  |

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 1311 | CD1 | LEU | 162 | 14.644 | 31.593 | -22.325 | 1.00 | 10.23 |
| ATOM | 1312 | CD2 | LEU | 162 | 16.390 | 33.093 | -23.326 | 1.00 | 10.26 |
| ATOM | 1313 | C   | LEU | 162 | 14.256 | 36.582 | -21.871 | 1.00 | 7.87  |
| ATOM | 1314 | O   | LEU | 162 | 14.228 | 37.234 | -22.926 | 1.00 | 8.10  |
| ATOM | 1315 | N   | ALA | 163 | 13.396 | 36.840 | -20.874 | 1.00 | 7.67  |
| ATOM | 1316 | CA  | ALA | 163 | 12.422 | 37.934 | -20.922 | 1.00 | 8.06  |
| ATOM | 1317 | CB  | ALA | 163 | 11.568 | 37.986 | -19.658 | 1.00 | 8.57  |
| ATOM | 1318 | C   | ALA | 163 | 13.122 | 39.278 | -21.162 | 1.00 | 8.14  |
| ATOM | 1319 | O   | ALA | 163 | 12.527 | 40.158 | -21.830 | 1.00 | 9.20  |
| ATOM | 1320 | N   | LEU | 164 | 14.320 | 39.445 | -20.607 | 1.00 | 8.56  |
| ATOM | 1321 | CA  | LEU | 164 | 15.075 | 40.688 | -20.710 | 1.00 | 8.69  |
| ATOM | 1322 | CB  | LEU | 164 | 15.881 | 40.917 | -19.409 | 1.00 | 9.34  |
| ATOM | 1323 | CG  | LEU | 164 | 15.007 | 41.231 | -18.199 | 1.00 | 9.92  |
| ATOM | 1324 | CD1 | LEU | 164 | 15.707 | 40.869 | -16.893 | 1.00 | 11.23 |
| ATOM | 1325 | CD2 | LEU | 164 | 14.532 | 42.665 | -18.193 | 1.00 | 11.47 |
| ATOM | 1326 | C   | LEU | 164 | 15.968 | 40.800 | -21.920 | 1.00 | 8.43  |
| ATOM | 1327 | O   | LEU | 164 | 16.728 | 41.751 | -22.068 | 1.00 | 10.53 |
| ATOM | 1328 | N   | GLY | 165 | 15.876 | 39.849 | -22.823 | 1.00 | 9.22  |
| ATOM | 1329 | CA  | GLY | 165 | 16.653 | 39.841 | -24.034 | 1.00 | 9.48  |
| ATOM | 1330 | C   | GLY | 165 | 18.044 | 39.299 | -23.843 | 1.00 | 9.17  |
| ATOM | 1331 | O   | GLY | 165 | 18.900 | 39.539 | -24.692 | 1.00 | 10.21 |
| ATOM | 1332 | N   | LYS | 166 | 18.298 | 38.579 | -22.754 | 1.00 | 9.48  |
| ATOM | 1333 | CA  | LYS | 166 | 19.627 | 38.033 | -22.452 | 1.00 | 9.96  |
| ATOM | 1334 | CB  | LYS | 166 | 19.982 | 38.274 | -20.984 | 1.00 | 9.69  |
| ATOM | 1335 | CG  | LYS | 166 | 19.946 | 39.708 | -20.549 | 1.00 | 11.03 |
| ATOM | 1336 | CD  | LYS | 166 | 20.825 | 40.606 | -21.352 | 1.00 | 14.43 |
| ATOM | 1337 | CE  | LYS | 166 | 20.799 | 42.029 | -20.820 | 1.00 | 18.44 |
| ATOM | 1338 | NZ  | LYS | 166 | 21.480 | 42.980 | -21.738 | 1.00 | 27.60 |
| ATOM | 1339 | C   | LYS | 166 | 19.669 | 36.535 | -22.725 | 1.00 | 9.64  |
| ATOM | 1340 | O   | LYS | 166 | 18.611 | 35.926 | -22.985 | 1.00 | 11.70 |
| ATOM | 1341 | N   | GLU | 167 | 20.837 | 35.917 | -22.660 | 1.00 | 9.56  |
| ATOM | 1342 | CA  | GLU | 167 | 20.979 | 34.447 | -22.758 | 1.00 | 10.09 |
| ATOM | 1343 | CB  | GLU | 167 | 22.436 | 34.051 | -22.993 | 1.00 | 12.65 |
| ATOM | 1344 | CG  | GLU | 167 | 23.380 | 34.300 | -21.838 | 1.00 | 22.48 |
| ATOM | 1345 | CD  | GLU | 167 | 23.665 | 33.149 | -20.891 | 1.00 | 25.40 |
| ATOM | 1346 | OE1 | GLU | 167 | 23.311 | 31.984 | -21.190 | 1.00 | 32.34 |
| ATOM | 1347 | OE2 | GLU | 167 | 24.326 | 33.330 | -19.840 | 1.00 | 31.11 |
| ATOM | 1348 | C   | GLU | 167 | 20.484 | 33.838 | -21.438 | 1.00 | 9.49  |
| ATOM | 1349 | O   | GLU | 167 | 20.519 | 34.524 | -20.407 | 1.00 | 10.35 |
| ATOM | 1350 | N   | GLU | 168 | 19.999 | 32.587 | -21.453 | 1.00 | 9.82  |
| ATOM | 1351 | CA  | GLU | 168 | 19.298 | 32.071 | -20.295 | 1.00 | 9.33  |
| ATOM | 1352 | CB  | GLU | 168 | 18.638 | 30.725 | -20.586 | 1.00 | 10.98 |
| ATOM | 1353 | CG  | GLU | 168 | 19.586 | 29.555 | -20.607 | 1.00 | 11.58 |
| ATOM | 1354 | CD  | GLU | 168 | 18.897 | 28.248 | -20.881 | 1.00 | 12.24 |
| ATOM | 1355 | OE1 | GLU | 168 | 19.518 | 27.191 | -20.621 | 1.00 | 16.73 |
| ATOM | 1356 | OE2 | GLU | 168 | 17.710 | 28.209 | -21.238 | 1.00 | 15.75 |
| ATOM | 1357 | C   | GLU | 168 | 20.121 | 31.991 | -19.021 | 1.00 | 9.76  |
| ATOM | 1358 | O   | GLU | 168 | 19.500 | 31.919 | -17.957 | 1.00 | 10.27 |
| ATOM | 1359 | N   | ASN | 169 | 21.440 | 31.959 | -19.098 | 1.00 | 11.16 |
| ATOM | 1360 | CA  | ASN | 169 | 22.256 | 31.849 | -17.894 | 1.00 | 11.83 |
| ATOM | 1361 | CB  | ASN | 169 | 23.467 | 30.962 | -18.200 | 1.00 | 17.37 |
| ATOM | 1362 | CG  | ASN | 169 | 23.037 | 29.534 | -18.442 | 1.00 | 25.58 |
| ATOM | 1363 | OD1 | ASN | 169 | 23.422 | 28.858 | -19.416 | 1.00 | 36.44 |
| ATOM | 1364 | ND2 | ASN | 169 | 22.234 | 29.059 | -17.485 | 1.00 | 33.88 |
| ATOM | 1365 | C   | ASN | 169 | 22.665 | 33.191 | -17.342 | 1.00 | 10.67 |
| ATOM | 1366 | O   | ASN | 169 | 23.471 | 33.254 | -16.423 | 1.00 | 10.87 |
| ATOM | 1367 | N   | PHE | 170 | 22.101 | 34.292 | -17.818 | 1.00 | 9.81  |
| ATOM | 1368 | CA  | PHE | 170 | 22.503 | 35.641 | -17.397 | 1.00 | 9.43  |
| ATOM | 1369 | CB  | PHE | 170 | 21.676 | 36.690 | -18.110 | 1.00 | 10.54 |
| ATOM | 1370 | CG  | PHE | 170 | 21.970 | 38.143 | -17.807 | 1.00 | 10.68 |
| ATOM | 1371 | CD1 | PHE | 170 | 22.971 | 38.748 | -18.561 | 1.00 | 11.73 |
| ATOM | 1372 | CD2 | PHE | 170 | 21.249 | 38.844 | -16.841 | 1.00 | 11.45 |
| ATOM | 1373 | CE1 | PHE | 170 | 23.277 | 40.069 | -18.325 | 1.00 | 13.22 |
| ATOM | 1374 | CE2 | PHE | 170 | 21.601 | 40.156 | -16.603 | 1.00 | 13.30 |
| ATOM | 1375 | CZ  | PHE | 170 | 22.581 | 40.787 | -17.369 | 1.00 | 13.73 |
| ATOM | 1376 | C   | PHE | 170 | 22.466 | 35.905 | -15.896 | 1.00 | 9.39  |
| ATOM | 1377 | O   | PHE | 170 | 23.388 | 36.499 | -15.313 | 1.00 | 10.53 |
| ATOM | 1378 | N   | PHE | 171 | 21.414 | 35.405 | -15.249 | 1.00 | 9.21  |
| ATOM | 1379 | CA  | PHE | 171 | 21.328 | 35.485 | -13.799 | 1.00 | 9.20  |
| ATOM | 1380 | CB  | PHE | 171 | 19.882 | 35.735 | -13.353 | 1.00 | 9.39  |
| ATOM | 1381 | CG  | PHE | 171 | 19.270 | 37.023 | -13.840 | 1.00 | 9.53  |
| ATOM | 1382 | CD1 | PHE | 171 | 18.199 | 36.958 | -14.716 | 1.00 | 8.43  |
| ATOM | 1383 | CD2 | PHE | 171 | 19.751 | 38.247 | -13.409 | 1.00 | 9.70  |

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 1384 | CE1 | PHE | 171 | 17.637 | 38.140 | -15.183 | 1.00 | 9.69  |
| ATOM | 1385 | CE2 | PHE | 171 | 19.208 | 39.427 | -13.881 | 1.00 | 11.03 |
| ATOM | 1386 | CZ  | PHE | 171 | 18.138 | 39.369 | -14.774 | 1.00 | 9.32  |
| ATOM | 1387 | C   | PHE | 171 | 21.798 | 34.187 | -13.158 | 1.00 | 9.45  |
| ATOM | 1388 | O   | PHE | 171 | 22.557 | 34.196 | -12.160 | 1.00 | 10.11 |
| ATOM | 1389 | N   | ALA | 172 | 21.386 | 33.058 | -13.727 | 1.00 | 8.64  |
| ATOM | 1390 | CA  | ALA | 172 | 21.662 | 31.758 | -13.141 | 1.00 | 9.25  |
| ATOM | 1391 | CB  | ALA | 172 | 20.995 | 30.619 | -13.907 | 1.00 | 11.46 |
| ATOM | 1392 | C   | ALA | 172 | 23.144 | 31.456 | -12.935 | 1.00 | 9.80  |
| ATOM | 1393 | O   | ALA | 172 | 23.515 | 30.728 | -12.017 | 1.00 | 9.88  |
| ATOM | 1394 | N   | ARG | 173 | 24.014 | 32.048 | -13.757 | 1.00 | 10.46 |
| ATOM | 1395 | CA  | ARG | 173 | 25.456 | 31.811 | -13.607 | 1.00 | 10.74 |
| ATOM | 1396 | CB  | ARG | 173 | 26.229 | 32.377 | -14.804 | 1.00 | 12.02 |
| ATOM | 1397 | CG  | ARG | 173 | 26.253 | 33.888 | -14.845 | 1.00 | 14.37 |
| ATOM | 1398 | CD  | ARG | 173 | 26.528 | 34.507 | -16.235 | 1.00 | 22.60 |
| ATOM | 1399 | NE  | ARG | 173 | 26.118 | 35.904 | -16.110 | 1.00 | 29.23 |
| ATOM | 1400 | CZ  | ARG | 173 | 26.204 | 37.054 | -16.666 | 1.00 | 27.71 |
| ATOM | 1401 | NH1 | ARG | 173 | 26.785 | 37.249 | -17.871 | 1.00 | 38.25 |
| ATOM | 1402 | NH2 | ARG | 173 | 25.671 | 38.128 | -16.092 | 1.00 | 20.56 |
| ATOM | 1403 | C   | ARG | 173 | 25.967 | 32.398 | -12.321 | 1.00 | 10.00 |
| ATOM | 1404 | O   | ARG | 173 | 27.059 | 31.984 | -11.891 | 1.00 | 12.18 |
| ATOM | 1405 | N   | HIS | 174 | 25.265 | 33.305 | -11.671 | 1.00 | 8.86  |
| ATOM | 1406 | CA  | HIS | 174 | 25.621 | 33.884 | -10.385 | 1.00 | 8.97  |
| ATOM | 1407 | CB  | HIS | 174 | 25.281 | 35.380 | -10.393 | 1.00 | 9.34  |
| ATOM | 1408 | CG  | HIS | 174 | 25.986 | 36.119 | -11.478 | 1.00 | 11.02 |
| ATOM | 1409 | CD2 | HIS | 174 | 27.271 | 36.548 | -11.356 | 1.00 | 13.05 |
| ATOM | 1410 | ND1 | HIS | 174 | 25.560 | 36.543 | -12.686 | 1.00 | 15.18 |
| ATOM | 1411 | CE1 | HIS | 174 | 26.532 | 37.180 | -13.306 | 1.00 | 16.14 |
| ATOM | 1412 | NE2 | HIS | 174 | 27.575 | 37.238 | -12.505 | 1.00 | 17.60 |
| ATOM | 1413 | C   | HIS | 174 | 24.864 | 33.267 | -9.203  | 1.00 | 8.17  |
| ATOM | 1414 | O   | HIS | 174 | 25.053 | 33.704 | -8.067  | 1.00 | 10.44 |
| ATOM | 1415 | N   | PHE | 175 | 24.093 | 32.251 | -9.482  | 1.00 | 8.57  |
| ATOM | 1416 | CA  | PHE | 175 | 23.230 | 31.536 | -8.516  | 1.00 | 7.07  |
| ATOM | 1417 | CB  | PHE | 175 | 21.772 | 31.678 | -8.967  | 1.00 | 7.09  |
| ATOM | 1418 | CG  | PHE | 175 | 20.743 | 31.096 | -8.020  | 1.00 | 6.00  |
| ATOM | 1419 | CD1 | PHE | 175 | 19.888 | 30.101 | -8.409  | 1.00 | 6.11  |
| ATOM | 1420 | CD2 | PHE | 175 | 20.644 | 31.566 | -6.725  | 1.00 | 6.48  |
| ATOM | 1421 | CE1 | PHE | 175 | 18.940 | 29.615 | -7.548  | 1.00 | 7.35  |
| ATOM | 1422 | CE2 | PHE | 175 | 19.709 | 31.073 | -5.837  | 1.00 | 7.65  |
| ATOM | 1423 | CZ  | PHE | 175 | 18.834 | 30.096 | -6.266  | 1.00 | 7.87  |
| ATOM | 1424 | C   | PHE | 175 | 23.686 | 30.089 | -8.421  | 1.00 | 7.96  |
| ATOM | 1425 | O   | PHE | 175 | 23.298 | 29.250 | -9.248  | 1.00 | 8.40  |
| ATOM | 1426 | N   | LYS | 176 | 24.602 | 29.813 | -7.494  | 1.00 | 7.81  |
| ATOM | 1427 | CA  | LYS | 176 | 25.320 | 28.576 | -7.473  | 1.00 | 7.94  |
| ATOM | 1428 | CB  | LYS | 176 | 26.813 | 28.901 | -7.674  | 1.00 | 10.84 |
| ATOM | 1429 | CG  | LYS | 176 | 27.215 | 29.556 | -8.956  | 1.00 | 15.51 |
| ATOM | 1430 | CD  | LYS | 176 | 28.584 | 30.190 | -8.877  | 1.00 | 23.52 |
| ATOM | 1431 | CE  | LYS | 176 | 28.905 | 31.261 | -7.886  | 1.00 | 31.75 |
| ATOM | 1432 | NZ  | LYS | 176 | 28.155 | 32.528 | -7.591  | 1.00 | 30.18 |
| ATOM | 1433 | C   | LYS | 176 | 25.206 | 27.890 | -6.114  | 1.00 | 7.44  |
| ATOM | 1434 | O   | LYS | 176 | 25.237 | 28.596 | -5.079  | 1.00 | 7.02  |
| ATOM | 1435 | N   | PRO | 177 | 25.115 | 26.568 | -6.114  | 1.00 | 7.06  |
| ATOM | 1436 | CD  | PRO | 177 | 25.016 | 25.639 | -7.241  | 1.00 | 8.87  |
| ATOM | 1437 | CA  | PRO | 177 | 24.978 | 25.874 | -4.841  | 1.00 | 7.22  |
| ATOM | 1438 | CB  | PRO | 177 | 24.960 | 24.392 | -5.244  | 1.00 | 9.12  |
| ATOM | 1439 | CG  | PRO | 177 | 24.494 | 24.351 | -6.632  | 1.00 | 12.20 |
| ATOM | 1440 | C   | PRO | 177 | 26.107 | 26.128 | -3.866  | 1.00 | 6.45  |
| ATOM | 1441 | O   | PRO | 177 | 25.842 | 26.133 | -2.655  | 1.00 | 6.96  |
| ATOM | 1442 | N   | ASP | 178 | 27.355 | 26.340 | -4.296  | 1.00 | 7.00  |
| ATOM | 1443 | CA  | ASP | 178 | 28.432 | 26.494 | -3.322  | 1.00 | 7.82  |
| ATOM | 1444 | CB  | ASP | 178 | 29.784 | 26.223 | -3.996  | 1.00 | 7.64  |
| ATOM | 1445 | CG  | ASP | 178 | 30.055 | 24.770 | -4.225  | 1.00 | 8.62  |
| ATOM | 1446 | OD1 | ASP | 178 | 29.305 | 23.888 | -3.752  | 1.00 | 10.49 |
| ATOM | 1447 | OD2 | ASP | 178 | 31.072 | 24.504 | -4.927  | 1.00 | 9.66  |
| ATOM | 1448 | C   | ASP | 178 | 28.418 | 27.826 | -2.624  | 1.00 | 8.41  |
| ATOM | 1449 | O   | ASP | 178 | 29.053 | 27.922 | -1.567  | 1.00 | 11.48 |
| ATOM | 1450 | N   | ASP | 179 | 27.747 | 28.844 | -3.172  | 1.00 | 7.61  |
| ATOM | 1451 | CA  | ASP | 179 | 27.868 | 30.160 | -2.558  | 1.00 | 8.48  |
| ATOM | 1452 | CB  | ASP | 179 | 29.017 | 31.003 | -3.110  | 1.00 | 14.39 |
| ATOM | 1453 | CG  | ASP | 179 | 28.896 | 31.215 | -4.582  | 1.00 | 17.08 |
| ATOM | 1454 | OD1 | ASP | 179 | 27.769 | 31.231 | -5.087  | 1.00 | 18.23 |
| ATOM | 1455 | OD2 | ASP | 179 | 29.974 | 31.247 | -5.214  | 1.00 | 29.01 |
| ATOM | 1456 | C   | ASP | 179 | 26.622 | 30.999 | -2.437  | 1.00 | 6.67  |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1457 | O   | ASP | 179 | 26.723 | 32.118 | -1.937 | 1.00 | 7.91  |
| ATOM | 1458 | N   | THR | 180 | 25.459 | 30.574 | -2.903 | 1.00 | 6.15  |
| ATOM | 1459 | CA  | THR | 180 | 24.291 | 31.397 | -2.818 | 1.00 | 5.45  |
| ATOM | 1460 | CB  | THR | 180 | 23.061 | 30.717 | -3.495 | 1.00 | 6.14  |
| ATOM | 1461 | OG1 | THR | 180 | 21.933 | 31.564 | -3.275 | 1.00 | 6.60  |
| ATOM | 1462 | CG2 | THR | 180 | 22.728 | 29.384 | -2.872 | 1.00 | 7.19  |
| ATOM | 1463 | C   | THR | 180 | 23.929 | 31.823 | -1.404 | 1.00 | 5.42  |
| ATOM | 1464 | O   | THR | 180 | 23.995 | 31.022 | -0.488 | 1.00 | 6.17  |
| ATOM | 1465 | N   | LEU | 181 | 23.568 | 33.098 | -1.291 | 1.00 | 5.82  |
| ATOM | 1466 | CA  | LEU | 181 | 23.100 | 33.709 | -0.086 | 1.00 | 5.33  |
| ATOM | 1467 | CB  | LEU | 181 | 23.535 | 35.173 | 0.000  | 1.00 | 5.68  |
| ATOM | 1468 | CG  | LEU | 181 | 25.031 | 35.342 | 0.214  | 1.00 | 7.12  |
| ATOM | 1469 | CD1 | LEU | 181 | 25.527 | 36.714 | -0.116 | 1.00 | 9.05  |
| ATOM | 1470 | CD2 | LEU | 181 | 25.431 | 34.952 | 1.631  | 1.00 | 9.04  |
| ATOM | 1471 | C   | LEU | 181 | 21.596 | 33.554 | 0.126  | 1.00 | 5.36  |
| ATOM | 1472 | O   | LEU | 181 | 21.002 | 34.159 | 1.018  | 1.00 | 5.78  |
| ATOM | 1473 | N   | ALA | 182 | 20.943 | 32.746 | -0.705 | 1.00 | 5.62  |
| ATOM | 1474 | CA  | ALA | 182 | 19.499 | 32.518 | -0.607 | 1.00 | 5.07  |
| ATOM | 1475 | CB  | ALA | 182 | 19.041 | 31.560 | -1.713 | 1.00 | 5.84  |
| ATOM | 1476 | C   | ALA | 182 | 19.111 | 31.916 | 0.741  | 1.00 | 5.26  |
| ATOM | 1477 | O   | ALA | 182 | 19.829 | 31.152 | 1.390  | 1.00 | 5.11  |
| ATOM | 1478 | N   | SER | 183 | 17.929 | 32.266 | 1.215  | 1.00 | 5.45  |
| ATOM | 1479 | CA  | SER | 183 | 17.387 | 31.766 | 2.475  | 1.00 | 5.43  |
| ATOM | 1480 | CB  | SER | 183 | 17.361 | 32.908 | 3.478  | 1.00 | 6.48  |
| ATOM | 1481 | OG  | SER | 183 | 16.484 | 33.920 | 3.050  | 1.00 | 7.39  |
| ATOM | 1482 | C   | SER | 183 | 15.975 | 31.229 | 2.287  | 1.00 | 5.28  |
| ATOM | 1483 | O   | SER | 183 | 15.220 | 31.691 | 1.430  | 1.00 | 5.14  |
| ATOM | 1484 | N   | VAL | 184 | 15.624 | 30.298 | 3.167  | 1.00 | 4.72  |
| ATOM | 1485 | CA  | VAL | 184 | 14.272 | 29.833 | 3.379  | 1.00 | 4.18  |
| ATOM | 1486 | CB  | VAL | 184 | 14.156 | 28.311 | 3.410  | 1.00 | 4.82  |
| ATOM | 1487 | CG1 | VAL | 184 | 12.784 | 27.827 | 3.825  | 1.00 | 5.78  |
| ATOM | 1488 | CG2 | VAL | 184 | 14.574 | 27.702 | 2.084  | 1.00 | 5.85  |
| ATOM | 1489 | C   | VAL | 184 | 13.803 | 30.392 | 4.728  | 1.00 | 4.63  |
| ATOM | 1490 | O   | VAL | 184 | 14.563 | 30.341 | 5.712  | 1.00 | 5.58  |
| ATOM | 1491 | N   | VAL | 185 | 12.571 | 30.872 | 4.785  | 1.00 | 5.40  |
| ATOM | 1492 | CA  | VAL | 185 | 11.960 | 31.260 | 6.049  | 1.00 | 5.11  |
| ATOM | 1493 | CB  | VAL | 185 | 11.732 | 32.758 | 6.222  | 1.00 | 5.44  |
| ATOM | 1494 | CG1 | VAL | 185 | 11.355 | 33.084 | 7.659  | 1.00 | 7.04  |
| ATOM | 1495 | CG2 | VAL | 185 | 12.974 | 33.556 | 5.824  | 1.00 | 7.05  |
| ATOM | 1496 | C   | VAL | 185 | 10.664 | 30.482 | 6.215  | 1.00 | 5.37  |
| ATOM | 1497 | O   | VAL | 185 | 9.793  | 30.537 | 5.354  | 1.00 | 6.79  |
| ATOM | 1498 | N   | LEU | 186 | 10.525 | 29.766 | 7.340  | 1.00 | 5.04  |
| ATOM | 1499 | CA  | LEU | 186 | 9.312  | 29.030 | 7.659  | 1.00 | 5.37  |
| ATOM | 1500 | CB  | LEU | 186 | 9.608  | 27.651 | 8.191  | 1.00 | 6.74  |
| ATOM | 1501 | CG  | LEU | 186 | 10.519 | 26.783 | 7.329  | 1.00 | 7.22  |
| ATOM | 1502 | CD1 | LEU | 186 | 10.783 | 25.457 | 8.026  | 1.00 | 8.08  |
| ATOM | 1503 | CD2 | LEU | 186 | 9.933  | 26.589 | 5.923  | 1.00 | 7.11  |
| ATOM | 1504 | C   | LEU | 186 | 8.512  | 29.883 | 8.645  | 1.00 | 5.24  |
| ATOM | 1505 | O   | LEU | 186 | 8.777  | 29.826 | 9.854  | 1.00 | 6.31  |
| ATOM | 1506 | N   | ILE | 187 | 7.577  | 30.701 | 8.165  | 1.00 | 5.56  |
| ATOM | 1507 | CA  | ILE | 187 | 6.864  | 31.641 | 9.010  | 1.00 | 5.65  |
| ATOM | 1508 | CB  | ILE | 187 | 6.589  | 32.984 | 8.305  | 1.00 | 6.04  |
| ATOM | 1509 | CG2 | ILE | 187 | 5.916  | 33.986 | 9.250  | 1.00 | 7.75  |
| ATOM | 1510 | CG1 | ILE | 187 | 7.804  | 33.601 | 7.633  | 1.00 | 6.80  |
| ATOM | 1511 | CD1 | ILE | 187 | 7.550  | 34.739 | 6.667  | 1.00 | 7.49  |
| ATOM | 1512 | C   | ILE | 187 | 5.511  | 31.068 | 9.440  | 1.00 | 6.09  |
| ATOM | 1513 | O   | ILE | 187 | 4.740  | 30.565 | 8.617  | 1.00 | 6.78  |
| ATOM | 1514 | N   | ARG | 188 | 5.253  | 31.145 | 10.736 | 1.00 | 6.56  |
| ATOM | 1515 | CA  | ARG | 188 | 3.970  | 30.800 | 11.332 | 1.00 | 6.28  |
| ATOM | 1516 | CB  | ARG | 188 | 4.130  | 29.967 | 12.611 | 1.00 | 7.38  |
| ATOM | 1517 | CG  | ARG | 188 | 2.799  | 29.623 | 13.245 | 1.00 | 7.70  |
| ATOM | 1518 | CD  | ARG | 188 | 2.926  | 29.038 | 14.641 | 1.00 | 9.29  |
| ATOM | 1519 | NE  | ARG | 188 | 1.588  | 28.821 | 15.185 | 1.00 | 11.11 |
| ATOM | 1520 | CZ  | ARG | 188 | 1.357  | 28.454 | 16.431 | 1.00 | 12.61 |
| ATOM | 1521 | NH1 | ARG | 188 | 2.357  | 28.232 | 17.264 | 1.00 | 16.10 |
| ATOM | 1522 | NH2 | ARG | 188 | 0.090  | 28.327 | 16.815 | 1.00 | 16.40 |
| ATOM | 1523 | C   | ARG | 188 | 3.224  | 32.081 | 11.714 | 1.00 | 6.29  |
| ATOM | 1524 | O   | ARG | 188 | 3.714  | 32.892 | 12.499 | 1.00 | 7.23  |
| ATOM | 1525 | N   | TYR | 189 | 2.053  | 32.239 | 11.099 | 1.00 | 6.43  |
| ATOM | 1526 | CA  | TYR | 189 | 1.129  | 33.301 | 11.534 | 1.00 | 6.36  |
| ATOM | 1527 | CB  | TYR | 189 | 0.565  | 33.997 | 10.302 | 1.00 | 7.87  |
| ATOM | 1528 | CG  | TYR | 189 | 1.432  | 35.109 | 9.770  | 1.00 | 7.69  |
| ATOM | 1529 | CD1 | TYR | 189 | 2.245  | 34.959 | 8.649  | 1.00 | 8.11  |

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|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1530 | CE1 | TYR | 189 | 3.023   | 36.028 | 8.202  | 1.00 | 8.55  |
| ATOM | 1531 | CD2 | TYR | 189 | 1.433   | 36.344 | 10.407 | 1.00 | 8.98  |
| ATOM | 1532 | CE2 | TYR | 189 | 2.188   | 37.415 | 9.969  | 1.00 | 9.17  |
| ATOM | 1533 | CZ  | TYR | 189 | 2.981   | 37.241 | 8.841  | 1.00 | 8.58  |
| ATOM | 1534 | OH  | TYR | 189 | 3.728   | 38.328 | 8.379  | 1.00 | 11.03 |
| ATOM | 1535 | C   | TYR | 189 | 0.033   | 32.562 | 12.300 | 1.00 | 7.25  |
| ATOM | 1536 | O   | TYR | 189 | -0.678  | 31.766 | 11.696 | 1.00 | 8.05  |
| ATOM | 1537 | N   | PRO | 190 | -0.137  | 32.811 | 13.576 | 1.00 | 6.97  |
| ATOM | 1538 | CD  | PRO | 190 | 0.666   | 33.760 | 14.412 | 1.00 | 7.48  |
| ATOM | 1539 | CA  | PRO | 190 | -1.091  | 32.037 | 14.367 | 1.00 | 7.93  |
| ATOM | 1540 | CB  | PRO | 190 | -0.484  | 32.215 | 15.773 | 1.00 | 9.03  |
| ATOM | 1541 | CG  | PRO | 190 | -0.032  | 33.667 | 15.732 | 1.00 | 8.65  |
| ATOM | 1542 | C   | PRO | 190 | -2.516  | 32.564 | 14.390 | 1.00 | 7.31  |
| ATOM | 1543 | O   | PRO | 190 | -2.768  | 33.746 | 14.183 | 1.00 | 7.83  |
| ATOM | 1544 | N   | TYR | 191 | -3.428  | 31.672 | 14.740 | 1.00 | 8.07  |
| ATOM | 1545 | CA  | TYR | 191 | -4.758  | 32.035 | 15.189 | 1.00 | 8.05  |
| ATOM | 1546 | CB  | TYR | 191 | -5.741  | 30.882 | 15.033 | 1.00 | 9.47  |
| ATOM | 1547 | CG  | TYR | 191 | -7.089  | 31.164 | 15.645 | 1.00 | 8.74  |
| ATOM | 1548 | CD1 | TYR | 191 | -7.981  | 32.032 | 15.052 | 1.00 | 10.94 |
| ATOM | 1549 | CE1 | TYR | 191 | -9.203  | 32.283 | 15.640 | 1.00 | 12.35 |
| ATOM | 1550 | CD2 | TYR | 191 | -7.434  | 30.628 | 16.867 | 1.00 | 11.98 |
| ATOM | 1551 | CE2 | TYR | 191 | -8.662  | 30.860 | 17.464 | 1.00 | 13.36 |
| ATOM | 1552 | CZ  | TYR | 191 | -9.520  | 31.710 | 16.847 | 1.00 | 13.52 |
| ATOM | 1553 | OH  | TYR | 191 | -10.758 | 31.949 | 17.411 | 1.00 | 20.40 |
| ATOM | 1554 | C   | TYR | 191 | -4.634  | 32.352 | 16.687 | 1.00 | 8.41  |
| ATOM | 1555 | O   | TYR | 191 | -4.028  | 31.574 | 17.419 | 1.00 | 10.11 |
| ATOM | 1556 | N   | LEU | 192 | -5.188  | 33.493 | 17.089 | 1.00 | 9.02  |
| ATOM | 1557 | CA  | LEU | 192 | -5.170  | 33.901 | 18.490 | 1.00 | 9.80  |
| ATOM | 1558 | CB  | LEU | 192 | -4.106  | 35.000 | 18.751 | 1.00 | 10.70 |
| ATOM | 1559 | CG  | LEU | 192 | -2.670  | 34.624 | 18.449 | 1.00 | 11.38 |
| ATOM | 1560 | CD1 | LEU | 192 | -1.779  | 35.835 | 18.366 | 1.00 | 15.17 |
| ATOM | 1561 | CD2 | LEU | 192 | -2.195  | 33.545 | 19.376 | 1.00 | 14.95 |
| ATOM | 1562 | C   | LEU | 192 | -6.524  | 34.466 | 18.870 | 1.00 | 11.59 |
| ATOM | 1563 | O   | LEU | 192 | -7.087  | 35.298 | 18.167 | 1.00 | 13.64 |
| ATOM | 1564 | N   | ASP | 193 | -7.038  | 34.106 | 20.036 | 1.00 | 14.51 |
| ATOM | 1565 | CA  | ASP | 193 | -8.305  | 34.590 | 20.567 | 1.00 | 17.44 |
| ATOM | 1566 | C   | ASP | 193 | -8.162  | 34.839 | 22.054 | 1.00 | 18.14 |
| ATOM | 1567 | O   | ASP | 193 | -8.094  | 33.884 | 22.833 | 1.00 | 20.69 |
| ATOM | 1568 | CB  | ASP | 193 | -9.424  | 33.558 | 20.361 | 1.00 | 19.90 |
| ATOM | 1569 | CG  | ASP | 193 | -10.778 | 34.035 | 20.844 | 1.00 | 22.56 |
| ATOM | 1570 | OD1 | ASP | 193 | -10.950 | 35.239 | 21.071 | 1.00 | 31.28 |
| ATOM | 1571 | OD2 | ASP | 193 | -11.705 | 33.195 | 20.904 | 1.00 | 31.66 |
| ATOM | 1572 | N   | PRO | 194 | -8.007  | 36.055 | 22.502 | 1.00 | 19.75 |
| ATOM | 1573 | CD  | PRO | 194 | -7.751  | 36.353 | 23.938 | 1.00 | 21.02 |
| ATOM | 1574 | CA  | PRO | 194 | -8.074  | 37.262 | 21.705 | 1.00 | 20.34 |
| ATOM | 1575 | CB  | PRO | 194 | -8.358  | 38.337 | 22.780 | 1.00 | 22.22 |
| ATOM | 1576 | CG  | PRO | 194 | -7.623  | 37.846 | 23.976 | 1.00 | 23.24 |
| ATOM | 1577 | C   | PRO | 194 | -6.794  | 37.553 | 20.961 | 1.00 | 18.30 |
| ATOM | 1578 | O   | PRO | 194 | -5.732  | 37.174 | 21.441 | 1.00 | 20.47 |
| ATOM | 1579 | N   | TYR | 195 | -6.908  | 38.261 | 19.844 | 1.00 | 16.09 |
| ATOM | 1580 | CA  | TYR | 195 | -5.729  | 38.654 | 19.057 | 1.00 | 13.39 |
| ATOM | 1581 | CB  | TYR | 195 | -6.063  | 38.748 | 17.591 | 1.00 | 11.89 |
| ATOM | 1582 | CG  | TYR | 195 | -4.857  | 38.589 | 16.678 | 1.00 | 10.40 |
| ATOM | 1583 | CD1 | TYR | 195 | -4.733  | 37.428 | 15.902 | 1.00 | 9.05  |
| ATOM | 1584 | CE1 | TYR | 195 | -3.668  | 37.229 | 15.052 | 1.00 | 9.43  |
| ATOM | 1585 | CD2 | TYR | 195 | -3.867  | 39.556 | 16.532 | 1.00 | 11.25 |
| ATOM | 1586 | CE2 | TYR | 195 | -2.801  | 39.370 | 15.678 | 1.00 | 10.47 |
| ATOM | 1587 | CZ  | TYR | 195 | -2.706  | 38.217 | 14.940 | 1.00 | 9.27  |
| ATOM | 1588 | OH  | TYR | 195 | -1.631  | 38.037 | 14.084 | 1.00 | 10.15 |
| ATOM | 1589 | C   | TYR | 195 | -5.251  | 40.015 | 19.570 | 1.00 | 16.02 |
| ATOM | 1590 | O   | TYR | 195 | -6.045  | 40.984 | 19.547 | 1.00 | 19.50 |
| ATOM | 1591 | N   | PRO | 196 | -4.015  | 40.101 | 20.038 | 1.00 | 19.81 |
| ATOM | 1592 | CD  | PRO | 196 | -2.943  | 39.107 | 19.944 | 1.00 | 20.75 |
| ATOM | 1593 | CA  | PRO | 196 | -3.555  | 41.366 | 20.632 | 1.00 | 22.65 |
| ATOM | 1594 | CB  | PRO | 196 | -2.113  | 41.061 | 21.050 | 1.00 | 24.78 |
| ATOM | 1595 | CG  | PRO | 196 | -1.702  | 39.919 | 20.178 | 1.00 | 25.22 |
| ATOM | 1596 | C   | PRO | 196 | -3.528  | 42.534 | 19.659 | 1.00 | 21.80 |
| ATOM | 1597 | O   | PRO | 196 | -2.893  | 42.411 | 18.610 | 1.00 | 18.33 |
| ATOM | 1598 | N   | ALA | 197 | -4.121  | 43.655 | 20.069 | 1.00 | 20.80 |
| ATOM | 1599 | CA  | ALA | 197 | -4.137  | 44.850 | 19.209 | 1.00 | 17.10 |
| ATOM | 1600 | CB  | ALA | 197 | -4.992  | 45.932 | 19.849 | 1.00 | 22.74 |
| ATOM | 1601 | C   | ALA | 197 | -2.736  | 45.332 | 18.943 | 1.00 | 16.42 |
| ATOM | 1602 | O   | ALA | 197 | -2.416  | 45.845 | 17.884 | 1.00 | 14.48 |

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|      |      |     |     |     |         |        |        |      |       |
|------|------|-----|-----|-----|---------|--------|--------|------|-------|
| ATOM | 1603 | N   | ALA | 198 | -1.806  | 45.093 | 19.872 | 1.00 | 18.94 |
| ATOM | 1604 | CA  | ALA | 198 | -0.457  | 45.551 | 19.663 | 1.00 | 18.82 |
| ATOM | 1605 | CB  | ALA | 198 | 0.389   | 45.537 | 20.917 | 1.00 | 21.76 |
| ATOM | 1606 | C   | ALA | 198 | 0.247   | 44.830 | 18.532 | 1.00 | 20.09 |
| ATOM | 1607 | O   | ALA | 198 | 1.209   | 45.380 | 17.989 | 1.00 | 20.87 |
| ATOM | 1608 | N   | ALA | 199 | -0.282  | 43.655 | 18.148 | 1.00 | 18.02 |
| ATOM | 1609 | CA  | ALA | 199 | 0.284   | 42.883 | 17.055 | 1.00 | 20.04 |
| ATOM | 1610 | CB  | ALA | 199 | 0.131   | 41.377 | 17.305 | 1.00 | 22.29 |
| ATOM | 1611 | C   | ALA | 199 | -0.405  | 43.201 | 15.745 | 1.00 | 17.65 |
| ATOM | 1612 | O   | ALA | 199 | -0.143  | 42.526 | 14.746 | 1.00 | 19.33 |
| ATOM | 1613 | N   | ILE | 200 | -1.272  | 44.187 | 15.758 | 1.00 | 14.55 |
| ATOM | 1614 | CA  | ILE | 200 | -2.007  | 44.619 | 14.572 | 1.00 | 12.89 |
| ATOM | 1615 | CB  | ILE | 200 | -3.524  | 44.490 | 14.735 | 1.00 | 12.11 |
| ATOM | 1616 | CG2 | ILE | 200 | -4.273  | 44.933 | 13.481 | 1.00 | 15.92 |
| ATOM | 1617 | CG1 | ILE | 200 | -3.933  | 43.079 | 15.169 | 1.00 | 12.87 |
| ATOM | 1618 | CD1 | ILE | 200 | -5.369  | 42.887 | 15.559 | 1.00 | 15.12 |
| ATOM | 1619 | C   | ILE | 200 | -1.604  | 46.049 | 14.242 | 1.00 | 12.80 |
| ATOM | 1620 | O   | ILE | 200 | -1.722  | 46.945 | 15.061 | 1.00 | 15.14 |
| ATOM | 1621 | N   | LYS | 201 | -1.079  | 46.217 | 13.030 | 1.00 | 12.46 |
| ATOM | 1622 | CA  | LYS | 201 | -0.723  | 47.561 | 12.585 | 1.00 | 13.42 |
| ATOM | 1623 | C   | LYS | 201 | -1.842  | 46.108 | 11.711 | 1.00 | 12.82 |
| ATOM | 1624 | O   | LYS | 201 | -2.682  | 47.341 | 11.198 | 1.00 | 12.98 |
| ATOM | 1625 | CB  | LYS | 201 | 0.575   | 47.555 | 11.793 | 1.00 | 15.55 |
| ATOM | 1626 | CG  | LYS | 201 | 1.786   | 47.469 | 12.720 | 1.00 | 22.73 |
| ATOM | 1627 | CD  | LYS | 201 | 2.968   | 47.442 | 11.792 | 1.00 | 30.21 |
| ATOM | 1628 | CE  | LYS | 201 | 3.330   | 45.969 | 11.633 | 1.00 | 33.55 |
| ATOM | 1629 | NZ  | LYS | 201 | 4.352   | 45.602 | 12.674 | 1.00 | 44.14 |
| ATOM | 1630 | N   | THR | 202 | -1.844  | 49.414 | 11.525 | 1.00 | 12.30 |
| ATOM | 1631 | CA  | THR | 202 | -2.896  | 50.018 | 10.731 | 1.00 | 12.03 |
| ATOM | 1632 | CB  | THR | 202 | -3.769  | 50.900 | 11.654 | 1.00 | 14.94 |
| ATOM | 1633 | OG1 | THR | 202 | -4.283  | 50.136 | 12.749 | 1.00 | 20.93 |
| ATOM | 1634 | CG2 | THR | 202 | -4.968  | 51.401 | 10.876 | 1.00 | 16.31 |
| ATOM | 1635 | C   | THR | 202 | -2.353  | 50.883 | 9.608  | 1.00 | 10.86 |
| ATOM | 1636 | O   | THR | 202 | -1.574  | 51.831 | 9.881  | 1.00 | 12.79 |
| ATOM | 1637 | N   | ALA | 203 | -2.710  | 50.593 | 8.362  | 1.00 | 10.61 |
| ATOM | 1638 | CA  | ALA | 203 | -2.246  | 51.412 | 7.251  | 1.00 | 10.61 |
| ATOM | 1639 | CB  | ALA | 203 | -2.554  | 50.704 | 5.923  | 1.00 | 10.92 |
| ATOM | 1640 | C   | ALA | 203 | -2.907  | 52.771 | 7.177  | 1.00 | 11.45 |
| ATOM | 1641 | O   | ALA | 203 | -3.927  | 53.003 | 7.798  | 1.00 | 12.75 |
| ATOM | 1642 | N   | ALA | 204 | -2.316  | 53.701 | 6.418  | 1.00 | 13.11 |
| ATOM | 1643 | CA  | ALA | 204 | -2.922  | 55.016 | 6.262  | 1.00 | 14.24 |
| ATOM | 1644 | CB  | ALA | 204 | -2.081  | 55.921 | 5.383  | 1.00 | 17.62 |
| ATOM | 1645 | C   | ALA | 204 | -4.312  | 54.951 | 5.666  | 1.00 | 15.18 |
| ATOM | 1646 | O   | ALA | 204 | -5.116  | 55.828 | 5.979  | 1.00 | 18.40 |
| ATOM | 1647 | N   | ASP | 205 | -4.656  | 53.935 | 4.910  | 1.00 | 14.70 |
| ATOM | 1648 | CA  | ASP | 205 | -6.010  | 53.765 | 4.378  | 1.00 | 15.08 |
| ATOM | 1649 | CB  | ASP | 205 | -5.939  | 53.130 | 2.979  | 1.00 | 14.53 |
| ATOM | 1650 | CG  | ASP | 205 | -5.558  | 51.681 | 2.919  | 1.00 | 13.86 |
| ATOM | 1651 | OD1 | ASP | 205 | -5.431  | 51.036 | 3.978  | 1.00 | 13.58 |
| ATOM | 1652 | OD2 | ASP | 205 | -5.414  | 51.137 | 1.785  | 1.00 | 14.56 |
| ATOM | 1653 | C   | ASP | 205 | -6.958  | 53.042 | 5.330  | 1.00 | 13.99 |
| ATOM | 1654 | O   | ASP | 205 | -8.100  | 52.729 | 4.944  | 1.00 | 16.91 |
| ATOM | 1655 | N   | GLY | 206 | -6.470  | 52.672 | 6.523  | 1.00 | 13.46 |
| ATOM | 1656 | CA  | GLY | 206 | -7.305  | 51.999 | 7.498  | 1.00 | 13.34 |
| ATOM | 1657 | C   | GLY | 206 | -7.215  | 50.496 | 7.536  | 1.00 | 12.65 |
| ATOM | 1658 | O   | GLY | 206 | -7.688  | 49.850 | 8.492  | 1.00 | 15.08 |
| ATOM | 1659 | N   | THR | 207 | -6.523  | 49.909 | 6.562  | 1.00 | 11.08 |
| ATOM | 1660 | CA  | THR | 207 | -6.383  | 48.461 | 6.501  | 1.00 | 10.33 |
| ATOM | 1661 | CB  | THR | 207 | -5.728  | 48.047 | 5.186  | 1.00 | 10.43 |
| ATOM | 1662 | OG1 | THR | 207 | -6.475  | 48.593 | 4.068  | 1.00 | 11.13 |
| ATOM | 1663 | CG2 | THR | 207 | -5.730  | 46.528 | 5.000  | 1.00 | 11.62 |
| ATOM | 1664 | C   | THR | 207 | -5.542  | 47.948 | 7.669  | 1.00 | 10.83 |
| ATOM | 1665 | O   | THR | 207 | -4.460  | 48.451 | 7.944  | 1.00 | 11.23 |
| ATOM | 1666 | N   | LYS | 208 | -6.047  | 46.906 | 8.322  | 1.00 | 10.43 |
| ATOM | 1667 | CA  | LYS | 208 | -5.328  | 46.251 | 9.393  | 1.00 | 10.06 |
| ATOM | 1668 | CB  | LYS | 208 | -6.299  | 45.472 | 10.281 | 1.00 | 10.90 |
| ATOM | 1669 | CG  | LYS | 208 | -7.310  | 46.400 | 10.977 | 1.00 | 15.45 |
| ATOM | 1670 | CD  | LYS | 208 | -8.216  | 45.550 | 11.860 | 1.00 | 21.10 |
| ATOM | 1671 | CE  | LYS | 208 | -9.070  | 46.277 | 12.858 | 1.00 | 25.92 |
| ATOM | 1672 | NZ  | LYS | 208 | -10.228 | 45.455 | 13.309 | 1.00 | 35.34 |
| ATOM | 1673 | C   | LYS | 208 | -4.281  | 45.341 | 8.753  | 1.00 | 8.69  |
| ATOM | 1674 | O   | LYS | 208 | -4.631  | 44.523 | 7.893  | 1.00 | 8.73  |
| ATOM | 1675 | N   | LEU | 209 | -3.058  | 45.470 | 9.211  | 1.00 | 8.66  |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1676 | CA  | LEU | 209 | -1.912 | 44.745 | 8.686  | 1.00 | 8.20  |
| ATOM | 1677 | CB  | LEU | 209 | -0.919 | 45.780 | 8.126  | 1.00 | 8.17  |
| ATOM | 1678 | CG  | LEU | 209 | -1.407 | 46.777 | 7.084  | 1.00 | 8.96  |
| ATOM | 1679 | CD1 | LEU | 209 | -0.263 | 47.711 | 6.737  | 1.00 | 10.26 |
| ATOM | 1680 | CD2 | LEU | 209 | -1.959 | 46.077 | 5.837  | 1.00 | 9.92  |
| ATOM | 1681 | C   | LEU | 209 | -1.149 | 43.969 | 9.733  | 1.00 | 8.39  |
| ATOM | 1682 | O   | LEU | 209 | -1.077 | 44.308 | 10.910 | 1.00 | 9.60  |
| ATOM | 1683 | N   | SER | 210 | -0.445 | 42.944 | 9.250  | 1.00 | 7.50  |
| ATOM | 1684 | CA  | SER | 210 | 0.555  | 42.241 | 10.017 | 1.00 | 8.27  |
| ATOM | 1685 | CB  | SER | 210 | 0.481  | 40.717 | 9.879  | 1.00 | 9.13  |
| ATOM | 1686 | OG  | SER | 210 | -0.677 | 40.154 | 10.458 | 1.00 | 10.38 |
| ATOM | 1687 | C   | SER | 210 | 1.958  | 42.709 | 9.625  | 1.00 | 8.82  |
| ATOM | 1688 | O   | SER | 210 | 2.867  | 42.559 | 10.430 | 1.00 | 11.07 |
| ATOM | 1689 | N   | PHE | 211 | 2.153  | 43.228 | 8.404  | 1.00 | 8.41  |
| ATOM | 1690 | CA  | PHE | 211 | 3.465  | 43.640 | 7.944  | 1.00 | 8.42  |
| ATOM | 1691 | CB  | PHE | 211 | 4.294  | 42.502 | 7.351  | 1.00 | 9.04  |
| ATOM | 1692 | CG  | PHE | 211 | 5.784  | 42.797 | 7.169  | 1.00 | 8.29  |
| ATOM | 1693 | CD1 | PHE | 211 | 6.656  | 42.844 | 8.237  | 1.00 | 9.90  |
| ATOM | 1694 | CD2 | PHE | 211 | 6.316  | 43.023 | 5.916  | 1.00 | 8.43  |
| ATOM | 1695 | CE1 | PHE | 211 | 8.014  | 43.064 | 8.074  | 1.00 | 9.71  |
| ATOM | 1696 | CE2 | PHE | 211 | 7.649  | 43.256 | 5.735  | 1.00 | 9.43  |
| ATOM | 1697 | CZ  | PHE | 211 | 8.515  | 43.240 | 6.804  | 1.00 | 8.86  |
| ATOM | 1698 | C   | PHE | 211 | 3.249  | 44.762 | 6.938  | 1.00 | 7.66  |
| ATOM | 1699 | O   | PHE | 211 | 2.415  | 44.662 | 6.051  | 1.00 | 8.72  |
| ATOM | 1700 | N   | GLU | 212 | 3.963  | 45.856 | 7.143  | 1.00 | 7.99  |
| ATOM | 1701 | CA  | GLU | 212 | 3.752  | 47.072 | 6.365  | 1.00 | 7.78  |
| ATOM | 1702 | CB  | GLU | 212 | 4.267  | 48.319 | 7.076  | 1.00 | 10.35 |
| ATOM | 1703 | CG  | GLU | 212 | 3.201  | 49.142 | 7.809  | 1.00 | 15.96 |
| ATOM | 1704 | CD  | GLU | 212 | 2.280  | 49.935 | 6.895  | 1.00 | 17.40 |
| ATOM | 1705 | OE1 | GLU | 212 | 1.606  | 50.866 | 7.415  | 1.00 | 19.49 |
| ATOM | 1706 | OE2 | GLU | 212 | 2.214  | 49.708 | 5.623  | 1.00 | 15.01 |
| ATOM | 1707 | C   | GLU | 212 | 4.328  | 46.972 | 4.954  | 1.00 | 7.86  |
| ATOM | 1708 | O   | GLU | 212 | 5.006  | 46.040 | 4.555  | 1.00 | 8.28  |
| ATOM | 1709 | N   | TRP | 213 | 3.992  | 47.997 | 4.162  | 1.00 | 8.57  |
| ATOM | 1710 | CA  | TRP | 213 | 4.464  | 48.141 | 2.806  | 1.00 | 8.31  |
| ATOM | 1711 | CB  | TRP | 213 | 3.999  | 49.421 | 2.155  | 1.00 | 8.34  |
| ATOM | 1712 | CG  | TRP | 213 | 4.620  | 50.707 | 2.603  | 1.00 | 9.80  |
| ATOM | 1713 | CD2 | TRP | 213 | 5.776  | 51.317 | 2.074  | 1.00 | 11.28 |
| ATOM | 1714 | CE2 | TRP | 213 | 5.977  | 52.520 | 2.784  | 1.00 | 12.37 |
| ATOM | 1715 | CE3 | TRP | 213 | 6.644  | 50.973 | 1.031  | 1.00 | 12.51 |
| ATOM | 1716 | CD1 | TRP | 213 | 4.181  | 51.522 | 3.610  | 1.00 | 10.15 |
| ATOM | 1717 | NE1 | TRP | 213 | 4.980  | 52.619 | 3.734  | 1.00 | 12.18 |
| ATOM | 1718 | CZ2 | TRP | 213 | 7.053  | 53.363 | 2.474  | 1.00 | 14.69 |
| ATOM | 1719 | CZ3 | TRP | 213 | 7.687  | 51.805 | 0.735  | 1.00 | 13.88 |
| ATOM | 1720 | CH2 | TRP | 213 | 7.887  | 52.990 | 1.460  | 1.00 | 15.53 |
| ATOM | 1721 | C   | TRP | 213 | 5.991  | 48.089 | 2.741  | 1.00 | 7.51  |
| ATOM | 1722 | O   | TRP | 213 | 6.720  | 48.548 | 3.592  | 1.00 | 8.44  |
| ATOM | 1723 | N   | HIS | 214 | 6.470  | 47.422 | 1.657  | 1.00 | 7.74  |
| ATOM | 1724 | CA  | HIS | 214 | 7.890  | 47.280 | 1.443  | 1.00 | 7.66  |
| ATOM | 1725 | CB  | HIS | 214 | 8.495  | 46.246 | 2.447  | 1.00 | 7.45  |
| ATOM | 1726 | CG  | HIS | 214 | 7.976  | 44.860 | 2.273  | 1.00 | 7.38  |
| ATOM | 1727 | CD2 | HIS | 214 | 8.527  | 43.765 | 1.682  | 1.00 | 7.28  |
| ATOM | 1728 | ND1 | HIS | 214 | 6.682  | 44.495 | 2.637  | 1.00 | 6.92  |
| ATOM | 1729 | CE1 | HIS | 214 | 6.501  | 43.234 | 2.298  | 1.00 | 7.44  |
| ATOM | 1730 | NE2 | HIS | 214 | 7.581  | 42.759 | 1.734  | 1.00 | 7.83  |
| ATOM | 1731 | C   | HIS | 214 | 8.125  | 46.789 | 0.014  | 1.00 | 6.97  |
| ATOM | 1732 | O   | HIS | 214 | 7.212  | 46.319 | -0.642 | 1.00 | 7.95  |
| ATOM | 1733 | N   | GLU | 215 | 9.384  | 46.910 | -0.408 | 1.00 | 7.78  |
| ATOM | 1734 | CA  | GLU | 215 | 9.921  | 46.216 | -1.569 | 1.00 | 8.05  |
| ATOM | 1735 | CB  | GLU | 215 | 10.780 | 47.140 | -2.413 | 1.00 | 9.46  |
| ATOM | 1736 | CG  | GLU | 215 | 10.056 | 48.276 | -3.051 | 1.00 | 11.54 |
| ATOM | 1737 | CD  | GLU | 215 | 10.919 | 49.189 | -3.900 | 1.00 | 16.19 |
| ATOM | 1738 | OE1 | GLU | 215 | 12.160 | 49.042 | -3.934 | 1.00 | 15.97 |
| ATOM | 1739 | OE2 | GLU | 215 | 10.349 | 50.051 | -4.616 | 1.00 | 23.46 |
| ATOM | 1740 | C   | GLU | 215 | 10.805 | 45.070 | -1.025 | 1.00 | 8.11  |
| ATOM | 1741 | O   | GLU | 215 | 11.385 | 45.184 | 0.071  | 1.00 | 8.95  |
| ATOM | 1742 | N   | ASP | 216 | 10.913 | 43.985 | -1.761 | 1.00 | 7.98  |
| ATOM | 1743 | CA  | ASP | 216 | 11.723 | 42.873 | -1.305 | 1.00 | 6.84  |
| ATOM | 1744 | CB  | ASP | 216 | 11.363 | 41.564 | -1.990 | 1.00 | 7.14  |
| ATOM | 1745 | CG  | ASP | 216 | 10.037 | 40.991 | -1.580 | 1.00 | 6.78  |
| ATOM | 1746 | OD1 | ASP | 216 | 9.415  | 41.594 | -0.693 | 1.00 | 7.44  |
| ATOM | 1747 | OD2 | ASP | 216 | 9.648  | 39.909 | -2.098 | 1.00 | 7.77  |
| ATOM | 1748 | C   | ASP | 216 | 13.214 | 43.128 | -1.469 | 1.00 | 6.24  |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1749 | O   | ASP | 216 | 13.696 | 43.704 | -2.450 | 1.00 | 7.93  |
| ATOM | 1750 | N   | VAL | 217 | 13.931 | 42.555 | -0.509 | 1.00 | 6.61  |
| ATOM | 1751 | CA  | VAL | 217 | 15.369 | 42.439 | -0.559 | 1.00 | 6.71  |
| ATOM | 1752 | CB  | VAL | 217 | 16.050 | 42.687 | 0.780  | 1.00 | 7.87  |
| ATOM | 1753 | CG1 | VAL | 217 | 17.568 | 42.640 | 0.641  | 1.00 | 9.01  |
| ATOM | 1754 | CG2 | VAL | 217 | 15.613 | 44.001 | 1.353  | 1.00 | 9.65  |
| ATOM | 1755 | C   | VAL | 217 | 15.714 | 41.072 | -1.150 | 1.00 | 6.75  |
| ATOM | 1756 | O   | VAL | 217 | 15.769 | 40.051 | -0.482 | 1.00 | 7.26  |
| ATOM | 1757 | N   | SER | 218 | 15.852 | 41.047 | -2.476 | 1.00 | 6.83  |
| ATOM | 1758 | CA  | SER | 218 | 16.056 | 39.850 | -3.257 | 1.00 | 6.43  |
| ATOM | 1759 | CB  | SER | 218 | 14.837 | 38.910 | -3.175 | 1.00 | 6.60  |
| ATOM | 1760 | OG  | SER | 218 | 13.749 | 39.472 | -3.890 | 1.00 | 6.81  |
| ATOM | 1761 | C   | SER | 218 | 16.304 | 40.211 | -4.722 | 1.00 | 5.92  |
| ATOM | 1762 | O   | SER | 218 | 16.044 | 41.351 | -5.112 | 1.00 | 6.97  |
| ATOM | 1763 | N   | LEU | 219 | 16.723 | 39.209 | -5.488 | 1.00 | 6.04  |
| ATOM | 1764 | CA  | LEU | 219 | 16.663 | 39.294 | -6.937 | 1.00 | 6.10  |
| ATOM | 1765 | CB  | LEU | 219 | 17.722 | 38.393 | -7.569 | 1.00 | 6.78  |
| ATOM | 1766 | CG  | LEU | 219 | 17.728 | 38.321 | -9.097 | 1.00 | 7.82  |
| ATOM | 1767 | CD1 | LEU | 219 | 18.034 | 39.650 | -9.731 | 1.00 | 9.76  |
| ATOM | 1768 | CD2 | LEU | 219 | 18.660 | 37.225 | -9.589 | 1.00 | 8.26  |
| ATOM | 1769 | C   | LEU | 219 | 15.218 | 36.982 | -7.341 | 1.00 | 5.92  |
| ATOM | 1770 | O   | LEU | 219 | 14.541 | 39.784 | -7.957 | 1.00 | 6.32  |
| ATOM | 1771 | N   | ILE | 220 | 14.743 | 37.780 | -6.965 | 1.00 | 5.60  |
| ATOM | 1772 | CA  | ILE | 220 | 13.342 | 37.411 | -7.010 | 1.00 | 5.79  |
| ATOM | 1773 | CB  | ILE | 220 | 12.950 | 36.552 | -8.228 | 1.00 | 6.51  |
| ATOM | 1774 | CG2 | ILE | 220 | 13.285 | 37.295 | -9.523 | 1.00 | 7.78  |
| ATOM | 1775 | CG1 | ILE | 220 | 13.563 | 35.144 | -8.189 | 1.00 | 6.95  |
| ATOM | 1776 | CD1 | ILE | 220 | 13.002 | 34.222 | -9.250 | 1.00 | 7.96  |
| ATOM | 1777 | C   | ILE | 220 | 12.977 | 36.695 | -5.712 | 1.00 | 5.16  |
| ATOM | 1778 | O   | ILE | 220 | 13.869 | 36.252 | -4.968 | 1.00 | 5.70  |
| ATOM | 1779 | N   | THR | 221 | 11.694 | 36.656 | -5.419 | 1.00 | 5.46  |
| ATOM | 1780 | CA  | THR | 221 | 11.121 | 35.981 | -4.263 | 1.00 | 6.07  |
| ATOM | 1781 | CB  | THR | 221 | 10.391 | 36.988 | -3.362 | 1.00 | 6.78  |
| ATOM | 1782 | OG1 | THR | 221 | 11.360 | 37.970 | -2.958 | 1.00 | 6.64  |
| ATOM | 1783 | CG2 | THR | 221 | 9.809  | 36.316 | -2.133 | 1.00 | 7.54  |
| ATOM | 1784 | C   | THR | 221 | 10.182 | 34.891 | -4.753 | 1.00 | 5.05  |
| ATOM | 1785 | O   | THR | 221 | 9.365  | 35.121 | -5.667 | 1.00 | 6.03  |
| ATOM | 1786 | N   | VAL | 222 | 10.317 | 33.704 | -4.181 | 1.00 | 5.43  |
| ATOM | 1787 | CA  | VAL | 222 | 9.635  | 32.477 | -4.589 | 1.00 | 5.29  |
| ATOM | 1788 | CB  | VAL | 222 | 10.610 | 31.467 | -5.188 | 1.00 | 5.74  |
| ATOM | 1789 | CG1 | VAL | 222 | 9.950  | 30.168 | -5.590 | 1.00 | 6.07  |
| ATOM | 1790 | CG2 | VAL | 222 | 11.389 | 32.046 | -6.358 | 1.00 | 6.22  |
| ATOM | 1791 | C   | VAL | 222 | 8.867  | 31.924 | -3.379 | 1.00 | 5.62  |
| ATOM | 1792 | O   | VAL | 222 | 9.466  | 31.333 | -2.465 | 1.00 | 5.72  |
| ATOM | 1793 | N   | LEU | 223 | 7.572  | 32.200 | -3.305 | 1.00 | 5.40  |
| ATOM | 1794 | CA  | LEU | 223 | 6.799  | 32.054 | -2.080 | 1.00 | 5.71  |
| ATOM | 1795 | CB  | LEU | 223 | 6.211  | 33.454 | -1.749 | 1.00 | 5.73  |
| ATOM | 1796 | CG  | LEU | 223 | 5.245  | 33.563 | -0.576 | 1.00 | 5.62  |
| ATOM | 1797 | CD1 | LEU | 223 | 5.992  | 33.305 | 0.748  | 1.00 | 5.34  |
| ATOM | 1798 | CD2 | LEU | 223 | 4.631  | 34.983 | -0.564 | 1.00 | 7.58  |
| ATOM | 1799 | C   | LEU | 223 | 5.672  | 31.053 | -2.119 | 1.00 | 5.89  |
| ATOM | 1800 | O   | LEU | 223 | 4.853  | 31.106 | -3.012 | 1.00 | 6.54  |
| ATOM | 1801 | N   | TYR | 224 | 5.637  | 30.185 | -1.112 | 1.00 | 5.35  |
| ATOM | 1802 | CA  | TYR | 224 | 4.493  | 29.307 | -0.858 | 1.00 | 5.93  |
| ATOM | 1803 | CB  | TYR | 224 | 4.891  | 27.865 | -0.543 | 1.00 | 7.37  |
| ATOM | 1804 | CG  | TYR | 224 | 3.696  | 27.082 | -0.030 | 1.00 | 8.60  |
| ATOM | 1805 | CD1 | TYR | 224 | 2.805  | 26.474 | -0.888 | 1.00 | 10.86 |
| ATOM | 1806 | CE1 | TYR | 224 | 1.698  | 25.762 | -0.350 | 1.00 | 11.92 |
| ATOM | 1807 | CD2 | TYR | 224 | 3.459  | 26.927 | 1.341  | 1.00 | 10.88 |
| ATOM | 1808 | CE2 | TYR | 224 | 2.363  | 26.334 | 1.897  | 1.00 | 12.37 |
| ATOM | 1809 | CZ  | TYR | 224 | 1.500  | 25.717 | 1.012  | 1.00 | 12.52 |
| ATOM | 1810 | OH  | TYR | 224 | 0.388  | 25.081 | 1.575  | 1.00 | 16.93 |
| ATOM | 1811 | C   | TYR | 224 | 3.702  | 29.956 | 0.284  | 1.00 | 5.19  |
| ATOM | 1812 | O   | TYR | 224 | 4.318  | 30.259 | 1.319  | 1.00 | 6.49  |
| ATOM | 1813 | N   | GLN | 225 | 2.391  | 29.993 | 0.209  | 1.00 | 5.70  |
| ATOM | 1814 | CA  | GLN | 225 | 1.552  | 30.327 | 1.336  | 1.00 | 6.51  |
| ATOM | 1815 | CB  | GLN | 225 | 1.053  | 31.753 | 1.362  | 1.00 | 8.15  |
| ATOM | 1816 | CG  | GLN | 225 | 2.113  | 32.840 | 1.196  | 1.00 | 8.18  |
| ATOM | 1817 | CD  | GLN | 225 | 1.591  | 34.205 | 1.582  | 1.00 | 8.60  |
| ATOM | 1818 | OE1 | GLN | 225 | 2.147  | 34.911 | 2.439  | 1.00 | 11.27 |
| ATOM | 1819 | NE2 | GLN | 225 | 0.536  | 34.580 | 0.927  | 1.00 | 9.01  |
| ATOM | 1820 | C   | GLN | 225 | 0.332  | 29.411 | 1.366  | 1.00 | 7.75  |
| ATOM | 1821 | O   | GLN | 225 | -0.163 | 28.937 | 0.352  | 1.00 | 8.52  |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1822 | N   | SER | 226 | -0.198 | 29.227 | 2.575  | 1.00 | 9.34  |
| ATOM | 1823 | CA  | SER | 226 | -1.464 | 28.544 | 2.758  | 1.00 | 10.96 |
| ATOM | 1824 | C2  | SER | 226 | -2.003 | 28.665 | 4.164  | 1.00 | 16.30 |
| ATOM | 1825 | OG  | SER | 226 | -1.115 | 28.419 | 5.120  | 1.00 | 15.06 |
| ATOM | 1826 | C   | SER | 226 | -2.559 | 29.310 | 2.014  | 1.00 | 10.35 |
| ATOM | 1827 | O   | SER | 226 | -2.481 | 30.484 | 1.699  | 1.00 | 11.80 |
| ATOM | 1828 | N   | ASN | 227 | -3.684 | 28.605 | 1.934  | 1.00 | 10.66 |
| ATOM | 1829 | CA  | ASN | 227 | -4.840 | 29.105 | 1.234  | 1.00 | 11.50 |
| ATOM | 1830 | CB  | ASN | 227 | -5.725 | 27.953 | 0.769  | 1.00 | 15.38 |
| ATOM | 1831 | CG  | ASN | 227 | -6.303 | 28.312 | -0.576 | 1.00 | 22.10 |
| ATOM | 1832 | OD1 | ASN | 227 | -6.033 | 27.643 | -1.583 | 1.00 | 35.45 |
| ATOM | 1833 | ND2 | ASN | 227 | -6.869 | 29.471 | -0.713 | 1.00 | 20.67 |
| ATOM | 1834 | C   | ASN | 227 | -5.668 | 30.072 | 2.070  | 1.00 | 12.61 |
| ATOM | 1835 | O   | ASN | 227 | -6.857 | 29.812 | 2.296  | 1.00 | 15.01 |
| ATOM | 1836 | N   | VAL | 228 | -5.078 | 31.162 | 2.514  | 1.00 | 10.77 |
| ATOM | 1837 | CA  | VAL | 228 | -5.746 | 32.223 | 3.268  | 1.00 | 9.90  |
| ATOM | 1838 | CB  | VAL | 228 | -5.417 | 32.224 | 4.768  | 1.00 | 11.72 |
| ATOM | 1839 | CG1 | VAL | 228 | -6.173 | 33.357 | 5.454  | 1.00 | 14.80 |
| ATOM | 1840 | CG2 | VAL | 228 | -5.721 | 30.872 | 5.403  | 1.00 | 14.80 |
| ATOM | 1841 | C   | VAL | 228 | -5.284 | 33.531 | 2.644  | 1.00 | 9.82  |
| ATOM | 1842 | O   | VAL | 228 | -4.093 | 33.821 | 2.657  | 1.00 | 10.96 |
| ATOM | 1843 | N   | GLN | 229 | -6.185 | 34.288 | 2.031  | 1.00 | 9.11  |
| ATOM | 1844 | CA  | GLN | 229 | -5.815 | 35.512 | 1.345  | 1.00 | 10.74 |
| ATOM | 1845 | CB  | GLN | 229 | -7.038 | 36.050 | 0.595  | 1.00 | 10.34 |
| ATOM | 1846 | CG  | GLN | 229 | -6.750 | 37.084 | -0.481 | 1.00 | 11.49 |
| ATOM | 1847 | CD  | GLN | 229 | -6.454 | 38.479 | 0.038  | 1.00 | 12.74 |
| ATOM | 1848 | OE1 | GLN | 229 | -7.057 | 38.953 | 1.011  | 1.00 | 10.77 |
| ATOM | 1849 | NE2 | GLN | 229 | -5.440 | 39.124 | -0.556 | 1.00 | 9.22  |
| ATOM | 1850 | C   | GLN | 229 | -5.228 | 36.489 | 2.340  | 1.00 | 10.98 |
| ATOM | 1851 | O   | GLN | 229 | -5.784 | 36.712 | 3.421  | 1.00 | 8.54  |
| ATOM | 1852 | N   | ASN | 230 | -4.133 | 37.140 | 1.924  | 1.00 | 9.75  |
| ATOM | 1853 | CA  | ASN | 230 | -3.504 | 38.106 | 2.839  | 1.00 | 10.52 |
| ATOM | 1854 | CB  | ASN | 230 | -2.642 | 37.356 | 3.865  | 1.00 | 11.42 |
| ATOM | 1855 | CG  | ASN | 230 | -1.468 | 36.649 | 3.229  | 1.00 | 12.95 |
| ATOM | 1856 | OD1 | ASN | 230 | -1.601 | 35.602 | 2.559  | 1.00 | 10.36 |
| ATOM | 1857 | ND2 | ASN | 230 | -0.321 | 37.258 | 3.367  | 1.00 | 9.22  |
| ATOM | 1858 | C   | ASN | 230 | -2.684 | 39.177 | 2.186  | 1.00 | 10.88 |
| ATOM | 1859 | O   | ASN | 230 | -2.579 | 40.278 | 2.699  | 1.00 | 8.35  |
| ATOM | 1860 | N   | LEU | 231 | -2.080 | 38.928 | 1.008  | 1.00 | 7.65  |
| ATOM | 1861 | CA  | LEU | 231 | -1.187 | 39.891 | 0.391  | 1.00 | 9.10  |
| ATOM | 1862 | CB  | LEU | 231 | -0.166 | 39.130 | -0.486 | 1.00 | 10.43 |
| ATOM | 1863 | CG  | LEU | 231 | 0.859  | 38.294 | 0.253  | 1.00 | 12.85 |
| ATOM | 1864 | CD1 | LEU | 231 | 1.718  | 37.494 | -0.719 | 1.00 | 18.74 |
| ATOM | 1865 | CD2 | LEU | 231 | 1.707  | 39.142 | 1.167  | 1.00 | 7.60  |
| ATOM | 1866 | C   | LEU | 231 | -1.921 | 40.933 | -0.444 | 1.00 | 8.69  |
| ATOM | 1867 | O   | LEU | 231 | -2.902 | 40.618 | -1.110 | 1.00 | 7.25  |
| ATOM | 1868 | N   | GLN | 232 | -1.378 | 42.167 | -0.446 | 1.00 | 8.77  |
| ATOM | 1869 | CA  | GLN | 232 | -1.884 | 43.212 | -1.298 | 1.00 | 10.24 |
| ATOM | 1870 | CB  | GLN | 232 | -2.611 | 44.274 | -0.523 | 1.00 | 11.66 |
| ATOM | 1871 | CG  | GLN | 232 | -3.852 | 43.777 | 0.218  | 1.00 | 14.46 |
| ATOM | 1872 | CD  | GLN | 232 | -4.616 | 44.915 | 0.825  | 1.00 | 6.81  |
| ATOM | 1873 | OE1 | GLN | 232 | -4.059 | 45.793 | 1.487  | 1.00 | 7.95  |
| ATOM | 1874 | NE2 | GLN | 232 | -5.935 | 44.904 | 0.648  | 1.00 | 7.9   |
| ATOM | 1875 | C   | GLN | 232 | -0.682 | 43.819 | -2.003 | 1.00 | 7.95  |
| ATOM | 1876 | O   | GLN | 232 | 0.375  | 43.965 | -1.390 | 1.00 | 7.92  |
| ATOM | 1877 | N   | VAL | 233 | -0.905 | 44.246 | -3.244 | 1.00 | 8.46  |
| ATOM | 1878 | CA  | VAL | 233 | 0.087  | 44.893 | -4.061 | 1.00 | 9.34  |
| ATOM | 1879 | CB  | VAL | 233 | 0.462  | 44.130 | -5.339 | 1.00 | 10.46 |
| ATOM | 1880 | CG1 | VAL | 233 | -0.719 | 43.775 | -6.224 | 1.00 | 9.44  |
| ATOM | 1881 | CG2 | VAL | 233 | 1.534  | 44.837 | -6.141 | 1.00 | 8.77  |
| ATOM | 1882 | C   | VAL | 233 | -0.381 | 46.307 | -4.399 | 1.00 | 12.76 |
| ATOM | 1883 | O   | VAL | 233 | -1.556 | 46.486 | -4.737 | 1.00 | 13.73 |
| ATOM | 1884 | N   | GLU | 234 | 0.489  | 47.302 | -4.314 | 1.00 | 8.62  |
| ATOM | 1885 | CA  | GLU | 234 | 0.169  | 48.654 | -4.763 | 1.00 | 10.41 |
| ATOM | 1886 | CB  | GLU | 234 | 1.095  | 49.693 | -4.115 | 1.00 | 11.08 |
| ATOM | 1887 | CG  | GLU | 234 | 0.638  | 51.126 | -4.319 | 1.00 | 12.14 |
| ATOM | 1888 | CD  | GLU | 234 | 1.488  | 52.093 | -3.531 | 1.00 | 13.51 |
| ATOM | 1889 | OE1 | GLU | 234 | 2.730  | 51.975 | -3.567 | 1.00 | 15.59 |
| ATOM | 1890 | OE2 | GLU | 234 | 0.903  | 53.025 | -2.925 | 1.00 | 17.29 |
| ATOM | 1891 | C   | GLU | 234 | 0.277  | 48.736 | -6.285 | 1.00 | 17.29 |
| ATOM | 1892 | O   | GLU | 234 | 1.295  | 48.366 | -6.885 | 1.00 | 13.51 |
| ATOM | 1893 | N   | THR | 235 | -0.753 | 49.285 | -6.917 | 1.00 | 15.59 |
| ATOM | 1894 | CA  | THR | 235 | -0.699 | 49.507 | -8.364 | 1.00 | 17.29 |

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 1895 | CB  | THR | 235 | -1.595 | 48.591 | -9.200  | 1.00 | 19.13 |
| ATOM | 1896 | OG1 | THR | 235 | -2.984 | 48.842 | -8.938  | 1.00 | 21.58 |
| ATOM | 1897 | CG2 | THR | 235 | -1.375 | 47.100 | -8.952  | 1.00 | 22.36 |
| ATOM | 1898 | C   | THR | 235 | -1.137 | 50.959 | -8.576  | 1.00 | 18.85 |
| ATOM | 1899 | O   | THR | 235 | -1.394 | 51.656 | -7.579  | 1.00 | 19.19 |
| ATOM | 1900 | N   | ALA | 236 | -1.293 | 51.330 | -9.856  | 1.00 | 22.89 |
| ATOM | 1901 | CA  | ALA | 236 | -1.784 | 52.664 | -10.222 | 1.00 | 23.88 |
| ATOM | 1902 | CB  | ALA | 236 | -1.749 | 52.884 | -11.725 | 1.00 | 31.13 |
| ATOM | 1903 | C   | ALA | 236 | -3.206 | 52.889 | -9.731  | 1.00 | 24.49 |
| ATOM | 1904 | O   | ALA | 236 | -3.723 | 53.962 | -9.427  | 1.00 | 31.36 |
| ATOM | 1905 | N   | ALA | 237 | -3.929 | 51.774 | -9.619  | 1.00 | 24.56 |
| ATOM | 1906 | CA  | ALA | 237 | -5.299 | 51.889 | -9.150  | 1.00 | 25.87 |
| ATOM | 1907 | CB  | ALA | 237 | -6.155 | 50.804 | -9.815  | 1.00 | 33.93 |
| ATOM | 1908 | C   | ALA | 237 | -5.332 | 51.715 | -7.648  | 1.00 | 24.45 |
| ATOM | 1909 | O   | ALA | 237 | -6.424 | 51.484 | -7.120  | 1.00 | 30.47 |
| ATOM | 1910 | N   | GLY | 238 | -4.223 | 51.758 | -6.932  | 1.00 | 21.71 |
| ATOM | 1911 | CA  | GLY | 238 | -4.269 | 51.563 | -5.481  | 1.00 | 19.83 |
| ATOM | 1912 | C   | GLY | 238 | -3.842 | 50.185 | -5.013  | 1.00 | 17.46 |
| ATOM | 1913 | O   | GLY | 238 | -3.387 | 49.372 | -5.837  | 1.00 | 17.96 |
| ATOM | 1914 | N   | TYR | 239 | -4.061 | 49.844 | -3.728  | 1.00 | 15.86 |
| ATOM | 1915 | CA  | TYR | 239 | -3.721 | 48.501 | -3.275  | 1.00 | 12.97 |
| ATOM | 1916 | CB  | TYR | 239 | -3.579 | 48.458 | -1.743  | 1.00 | 12.30 |
| ATOM | 1917 | CG  | TYR | 239 | -2.235 | 48.936 | -1.252  | 1.00 | 11.99 |
| ATOM | 1918 | CD1 | TYR | 239 | -2.034 | 50.267 | -0.939  | 1.00 | 12.25 |
| ATOM | 1919 | CE1 | TYR | 239 | -0.787 | 50.701 | -0.501  | 1.00 | 12.55 |
| ATOM | 1920 | CD2 | TYR | 239 | -1.161 | 48.056 | -1.168  | 1.00 | 11.54 |
| ATOM | 1921 | CE2 | TYR | 239 | 0.072  | 48.470 | -0.746  | 1.00 | 11.38 |
| ATOM | 1922 | CZ  | TYR | 239 | 0.238  | 49.811 | -0.426  | 1.00 | 11.23 |
| ATOM | 1923 | OH  | TYR | 239 | 1.484  | 50.235 | -0.015  | 1.00 | 14.40 |
| ATOM | 1924 | C   | TYR | 239 | -4.815 | 47.516 | -3.705  | 1.00 | 12.53 |
| ATOM | 1925 | O   | TYR | 239 | -6.007 | 47.800 | -3.513  | 1.00 | 17.24 |
| ATOM | 1926 | N   | GLN | 240 | -4.409 | 46.398 | -4.296  | 1.00 | 11.52 |
| ATOM | 1927 | CA  | GLN | 240 | -5.297 | 45.349 | -4.769  | 1.00 | 11.73 |
| ATOM | 1928 | CB  | GLN | 240 | -5.117 | 45.199 | -6.306  | 1.00 | 11.64 |
| ATOM | 1929 | CG  | GLN | 240 | -5.539 | 46.485 | -7.051  | 1.00 | 14.46 |
| ATOM | 1930 | CD  | GLN | 240 | -5.418 | 46.379 | -8.546  | 1.00 | 16.63 |
| ATOM | 1931 | OE1 | GLN | 240 | -4.585 | 45.635 | -9.069  | 1.00 | 18.79 |
| ATOM | 1932 | NE2 | GLN | 240 | -6.217 | 47.136 | -9.296  | 1.00 | 21.51 |
| ATOM | 1933 | C   | GLN | 240 | -4.935 | 44.026 | -4.113  | 1.00 | 10.88 |
| ATOM | 1934 | O   | GLN | 240 | -3.763 | 43.770 | -3.789  | 1.00 | 9.92  |
| ATOM | 1935 | N   | ASP | 241 | -5.922 | 43.182 | -3.859  | 1.00 | 10.67 |
| ATOM | 1936 | CA  | ASP | 241 | -5.711 | 41.915 | -3.230  | 1.00 | 9.82  |
| ATOM | 1937 | CB  | ASP | 241 | -7.072 | 41.409 | -2.727  | 1.00 | 11.01 |
| ATOM | 1938 | CG  | ASP | 241 | -7.532 | 41.987 | -1.420  | 1.00 | 12.59 |
| ATOM | 1939 | OD1 | ASP | 241 | -8.763 | 41.911 | -1.141  | 1.00 | 15.81 |
| ATOM | 1940 | OD2 | ASP | 241 | -6.719 | 42.478 | -0.648  | 1.00 | 12.84 |
| ATOM | 1941 | C   | ASP | 241 | -5.124 | 40.876 | -4.183  | 1.00 | 10.03 |
| ATOM | 1942 | O   | ASP | 241 | -5.613 | 40.615 | -5.276  | 1.00 | 13.99 |
| ATOM | 1943 | N   | ILE | 242 | -4.082 | 40.170 | -3.742  | 1.00 | 8.45  |
| ATOM | 1944 | CA  | ILE | 242 | -3.524 | 39.035 | -4.454  | 1.00 | 8.44  |
| ATOM | 1945 | CB  | ILE | 242 | -2.024 | 38.896 | -4.197  | 1.00 | 8.68  |
| ATOM | 1946 | CG2 | ILE | 242 | -1.499 | 37.564 | -4.760  | 1.00 | 10.88 |
| ATOM | 1947 | CG1 | ILE | 242 | -1.271 | 40.096 | -4.766  | 1.00 | 9.70  |
| ATOM | 1948 | CD1 | ILE | 242 | 0.191  | 40.223 | -4.344  | 1.00 | 11.78 |
| ATOM | 1949 | C   | ILE | 242 | -4.242 | 37.784 | -3.942  | 1.00 | 8.96  |
| ATOM | 1950 | O   | ILE | 242 | -4.216 | 37.474 | -2.740  | 1.00 | 9.65  |
| ATOM | 1951 | N   | ALA | 243 | -4.926 | 37.054 | -4.821  | 1.00 | 9.75  |
| ATOM | 1952 | CA  | ALA | 243 | -5.595 | 35.814 | -4.414  | 1.00 | 9.73  |
| ATOM | 1953 | C   | ALA | 243 | -4.574 | 34.776 | -3.950  | 1.00 | 8.94  |
| ATOM | 1954 | O   | ALA | 243 | -3.463 | 34.685 | -4.478  | 1.00 | 11.10 |
| ATOM | 1955 | CB  | ALA | 243 | -6.379 | 35.243 | -5.605  | 1.00 | 14.74 |
| ATOM | 1956 | N   | ALA | 244 | -4.991 | 33.948 | -2.985  | 1.00 | 9.36  |
| ATOM | 1957 | CA  | ALA | 244 | -4.136 | 32.844 | -2.547  | 1.00 | 9.36  |
| ATOM | 1958 | CB  | ALA | 244 | -4.588 | 32.409 | -1.156  | 1.00 | 13.93 |
| ATOM | 1959 | C   | ALA | 244 | -4.243 | 31.707 | -3.540  | 1.00 | 10.49 |
| ATOM | 1960 | O   | ALA | 244 | -5.263 | 31.547 | -4.224  | 1.00 | 13.13 |
| ATOM | 1961 | N   | ASP | 245 | -3.215 | 30.899 | -3.615  | 1.00 | 10.92 |
| ATOM | 1962 | CA  | ASP | 245 | -3.158 | 29.661 | -4.408  | 1.00 | 11.37 |
| ATOM | 1963 | CB  | ASP | 245 | -2.804 | 29.876 | -5.858  | 1.00 | 11.89 |
| ATOM | 1964 | CG  | ASP | 245 | -2.892 | 28.664 | -6.747  | 1.00 | 13.54 |
| ATOM | 1965 | OD1 | ASP | 245 | -3.031 | 28.761 | -7.996  | 1.00 | 18.77 |
| ATOM | 1966 | OD2 | ASP | 245 | -2.886 | 27.549 | -6.197  | 1.00 | 13.74 |
| ATOM | 1967 | C   | ASP | 245 | -2.109 | 28.779 | -3.720  | 1.00 | 10.46 |

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 1968 | O   | ASP | 245 | -0.917 | 28.912 | -3.998  | 1.00 | 11.30 |
| ATOM | 1969 | N   | ASP | 246 | -2.562 | 27.850 | -2.905  | 1.00 | 9.06  |
| ATOM | 1970 | CA  | ASP | 246 | -1.677 | 26.921 | -2.197  | 1.00 | 9.74  |
| ATOM | 1971 | CB  | ASP | 246 | -2.253 | 26.499 | -0.859  | 1.00 | 11.33 |
| ATOM | 1972 | CG  | ASP | 246 | -3.378 | 25.495 | -1.011  | 1.00 | 13.92 |
| ATOM | 1973 | OD1 | ASP | 246 | -3.834 | 24.958 | 0.018   | 1.00 | 15.40 |
| ATOM | 1974 | OD2 | ASP | 246 | -3.870 | 25.292 | -2.155  | 1.00 | 14.85 |
| ATOM | 1975 | C   | ASP | 246 | -1.201 | 25.755 | -3.060  | 1.00 | 9.71  |
| ATOM | 1976 | O   | ASP | 246 | -0.571 | 24.838 | -2.544  | 1.00 | 10.59 |
| ATOM | 1977 | N   | THR | 247 | -1.417 | 25.840 | -4.379  | 1.00 | 9.46  |
| ATOM | 1978 | CA  | THR | 247 | -0.834 | 24.865 | -5.261  | 1.00 | 9.37  |
| ATOM | 1979 | CB  | THR | 247 | -1.845 | 24.275 | -6.269  | 1.00 | 11.29 |
| ATOM | 1980 | OG1 | THR | 247 | -2.235 | 25.290 | -7.212  | 1.00 | 11.39 |
| ATOM | 1981 | CG2 | THR | 247 | -3.094 | 23.800 | -5.524  | 1.00 | 12.30 |
| ATOM | 1982 | C   | THR | 247 | 0.328  | 25.442 | -6.058  | 1.00 | 8.75  |
| ATOM | 1983 | O   | THR | 247 | 1.026  | 24.639 | -6.698  | 1.00 | 11.70 |
| ATOM | 1984 | N   | GLY | 248 | 0.477  | 26.744 | -6.088  | 1.00 | 8.16  |
| ATOM | 1985 | CA  | GLY | 248 | 1.475  | 27.454 | -6.872  | 1.00 | 8.53  |
| ATOM | 1986 | C   | GLY | 248 | 2.494  | 28.172 | -5.992  | 1.00 | 7.49  |
| ATOM | 1987 | O   | GLY | 248 | 2.373  | 28.246 | -4.757  | 1.00 | 10.66 |
| ATOM | 1988 | N   | TYR | 249 | 3.496  | 28.733 | -6.663  | 1.00 | 6.67  |
| ATOM | 1989 | CA  | TYR | 249 | 4.437  | 29.616 | -6.005  | 1.00 | 6.51  |
| ATOM | 1990 | CB  | TYR | 249 | 5.900  | 29.244 | -6.303  | 1.00 | 6.70  |
| ATOM | 1991 | CG  | TYR | 249 | 6.411  | 28.129 | -5.426  | 1.00 | 6.10  |
| ATOM | 1992 | CD1 | TYR | 249 | 6.314  | 26.788 | -5.752  | 1.00 | 6.62  |
| ATOM | 1993 | CE1 | TYR | 249 | 6.786  | 25.803 | -4.929  | 1.00 | 7.14  |
| ATOM | 1994 | CD2 | TYR | 249 | 6.992  | 28.437 | -4.199  | 1.00 | 5.64  |
| ATOM | 1995 | CE2 | TYR | 249 | 7.470  | 27.450 | -3.364  | 1.00 | 5.23  |
| ATOM | 1996 | CZ  | TYR | 249 | 7.367  | 26.135 | -3.715  | 1.00 | 6.30  |
| ATOM | 1997 | OH  | TYR | 249 | 7.823  | 25.130 | -2.903  | 1.00 | 8.55  |
| ATOM | 1998 | C   | TYR | 249 | 4.202  | 31.046 | -6.523  | 1.00 | 5.67  |
| ATOM | 1999 | O   | TYR | 249 | 4.146  | 31.252 | -7.740  | 1.00 | 6.93  |
| ATOM | 2000 | N   | LEU | 250 | 4.045  | 31.976 | -5.592  | 1.00 | 5.56  |
| ATOM | 2001 | CA  | LEU | 250 | 3.894  | 33.381 | -5.926  | 1.00 | 5.35  |
| ATOM | 2002 | CB  | LEU | 250 | 3.151  | 34.119 | -4.803  | 1.00 | 6.61  |
| ATOM | 2003 | CG  | LEU | 250 | 2.830  | 35.587 | -5.134  | 1.00 | 6.78  |
| ATOM | 2004 | CD1 | LEU | 250 | 1.810  | 35.727 | -6.251  | 1.00 | 7.40  |
| ATOM | 2005 | CD2 | LEU | 250 | 2.316  | 36.240 | -3.857  | 1.00 | 8.54  |
| ATOM | 2006 | C   | LEU | 250 | 5.283  | 33.945 | -6.147  | 1.00 | 5.86  |
| ATOM | 2007 | O   | LEU | 250 | 6.157  | 33.797 | -5.272  | 1.00 | 5.91  |
| ATOM | 2008 | N   | ILE | 251 | 5.498  | 34.540 | -7.312  | 1.00 | 5.45  |
| ATOM | 2009 | CA  | ILE | 251 | 6.777  | 35.088 | -7.727  | 1.00 | 6.03  |
| ATOM | 2010 | CB  | ILE | 251 | 7.240  | 34.434 | -9.059  | 1.00 | 6.08  |
| ATOM | 2011 | CG2 | ILE | 251 | 8.728  | 34.801 | -9.306  | 1.00 | 7.80  |
| ATOM | 2012 | CG1 | ILE | 251 | 6.975  | 32.941 | -9.095  | 1.00 | 5.58  |
| ATOM | 2013 | CD1 | ILE | 251 | 7.657  | 32.110 | -8.038  | 1.00 | 6.65  |
| ATOM | 2014 | C   | ILE | 251 | 6.712  | 36.599 | -7.909  | 1.00 | 6.10  |
| ATOM | 2015 | O   | ILE | 251 | 5.735  | 37.111 | -8.484  | 1.00 | 6.96  |
| ATOM | 2016 | N   | ASN | 252 | 7.760  | 37.291 | -7.443  | 1.00 | 6.11  |
| ATOM | 2017 | CA  | ASN | 252 | 7.892  | 38.703 | -7.696  | 1.00 | 6.61  |
| ATOM | 2018 | CB  | ASN | 252 | 7.145  | 39.615 | -6.739  | 1.00 | 7.62  |
| ATOM | 2019 | CG  | ASN | 252 | 7.617  | 39.521 | -5.306  | 1.00 | 8.27  |
| ATOM | 2020 | OD1 | ASN | 252 | 7.166  | 38.626 | -4.587  | 1.00 | 9.37  |
| ATOM | 2021 | ND2 | ASN | 252 | 8.520  | 40.387 | -4.902  | 1.00 | 8.45  |
| ATOM | 2022 | C   | ASN | 252 | 9.377  | 39.065 | -7.731  | 1.00 | 6.35  |
| ATOM | 2023 | O   | ASN | 252 | 10.197 | 38.345 | -7.137  | 1.00 | 7.21  |
| ATOM | 2024 | N   | CYS | 253 | 9.683  | 40.236 | -8.295  | 1.00 | 6.40  |
| ATOM | 2025 | CA  | CYS | 253 | 11.048 | 40.768 | -8.285  | 1.00 | 7.03  |
| ATOM | 2026 | CB  | CYS | 253 | 11.302 | 41.723 | -9.464  | 1.00 | 8.85  |
| ATOM | 2027 | SG  | CYS | 253 | 11.232 | 40.881 | -11.077 | 1.00 | 10.36 |
| ATOM | 2028 | C   | CYS | 253 | 11.309 | 41.552 | -6.988  | 1.00 | 7.30  |
| ATOM | 2029 | O   | CYS | 253 | 10.402 | 42.203 | -6.420  | 1.00 | 7.55  |
| ATOM | 2030 | N   | GLY | 254 | 12.562 | 41.539 | -6.585  | 1.00 | 6.67  |
| ATOM | 2031 | CA  | GLY | 254 | 13.063 | 42.360 | -5.503  | 1.00 | 7.05  |
| ATOM | 2032 | C   | GLY | 254 | 13.850 | 43.536 | -6.046  | 1.00 | 7.09  |
| ATOM | 2033 | O   | GLY | 254 | 14.011 | 43.696 | -7.269  | 1.00 | 7.78  |
| ATOM | 2034 | N   | SER | 255 | 14.338 | 44.380 | -5.130  | 1.00 | 7.39  |
| ATOM | 2035 | CA  | SER | 255 | 14.942 | 45.634 | -5.560  | 1.00 | 8.33  |
| ATOM | 2036 | CB  | SER | 255 | 14.980 | 46.646 | -4.420  | 1.00 | 8.09  |
| ATOM | 2037 | OG  | SER | 255 | 15.785 | 46.124 | -3.385  | 1.00 | 9.54  |
| ATOM | 2038 | C   | SER | 255 | 16.275 | 45.443 | -6.277  | 1.00 | 7.85  |
| ATOM | 2039 | O   | SER | 255 | 16.710 | 46.348 | -6.979  | 1.00 | 10.10 |
| ATOM | 2040 | N   | TYR | 256 | 16.928 | 44.287 | -6.184  | 1.00 | 7.83  |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2041 | CA  | TYR | 256 | 18.151 | 44.106 | -6.964  | 1.00 | 8.12  |
| ATOM | 2042 | CB  | TYR | 256 | 18.966 | 42.909 | -6.486  | 1.00 | 7.96  |
| ATOM | 2043 | CG  | TYR | 256 | 20.395 | 42.919 | -7.017  | 1.00 | 7.92  |
| ATOM | 2044 | CD1 | TYR | 256 | 21.351 | 43.735 | -6.425  | 1.00 | 9.18  |
| ATOM | 2045 | CE1 | TYR | 256 | 22.665 | 43.731 | -6.866  | 1.00 | 9.56  |
| ATOM | 2046 | CD2 | TYR | 256 | 20.800 | 42.110 | -8.068  | 1.00 | 8.38  |
| ATOM | 2047 | CE2 | TYR | 256 | 22.119 | 42.114 | -8.530  | 1.00 | 8.77  |
| ATOM | 2048 | CZ  | TYR | 256 | 23.030 | 42.931 | -7.942  | 1.00 | 7.91  |
| ATOM | 2049 | OH  | TYR | 256 | 24.334 | 42.919 | -8.446  | 1.00 | 10.55 |
| ATOM | 2050 | C   | TYR | 256 | 17.790 | 44.007 | -8.444  | 1.00 | 7.77  |
| ATOM | 2051 | O   | TYR | 256 | 18.510 | 44.559 | -9.307  | 1.00 | 9.14  |
| ATOM | 2052 | N   | MET | 257 | 16.689 | 43.310 | -8.767  | 1.00 | 8.12  |
| ATOM | 2053 | CA  | MET | 257 | 16.220 | 43.230 | -10.151 | 1.00 | 7.70  |
| ATOM | 2054 | CB  | MET | 257 | 15.002 | 42.301 | -10.305 | 1.00 | 8.40  |
| ATOM | 2055 | CG  | MET | 257 | 14.582 | 42.102 | -11.738 | 1.00 | 9.02  |
| ATOM | 2056 | SD  | MET | 257 | 15.730 | 41.115 | -12.738 | 1.00 | 9.56  |
| ATOM | 2057 | CE  | MET | 257 | 15.233 | 39.485 | -12.131 | 1.00 | 11.37 |
| ATOM | 2058 | C   | MET | 257 | 15.843 | 44.629 | -10.670 | 1.00 | 6.94  |
| ATOM | 2059 | O   | MET | 257 | 16.150 | 44.976 | -11.819 | 1.00 | 8.48  |
| ATOM | 2060 | N   | ALA | 258 | 15.189 | 45.427 | -9.842  | 1.00 | 7.83  |
| ATOM | 2061 | CA  | ALA | 258 | 14.807 | 46.786 | -10.242 | 1.00 | 8.49  |
| ATOM | 2062 | CB  | ALA | 258 | 13.940 | 47.433 | -9.204  | 1.00 | 8.60  |
| ATOM | 2063 | C   | ALA | 258 | 16.074 | 47.582 | -10.550 | 1.00 | 8.95  |
| ATOM | 2064 | O   | ALA | 258 | 15.128 | 48.339 | -11.526 | 1.00 | 10.68 |
| ATOM | 2065 | N   | HIS | 259 | 17.075 | 47.456 | -9.717  | 1.00 | 9.55  |
| ATOM | 2066 | CA  | HIS | 259 | 18.325 | 48.184 | -9.987  | 1.00 | 9.84  |
| ATOM | 2067 | CB  | HIS | 259 | 19.298 | 47.968 | -8.806  | 1.00 | 10.82 |
| ATOM | 2068 | CG  | HIS | 259 | 20.581 | 48.672 | -8.960  | 1.00 | 12.01 |
| ATOM | 2069 | CD2 | HIS | 259 | 20.785 | 50.004 | -8.919  | 1.00 | 11.84 |
| ATOM | 2070 | ND1 | HIS | 259 | 21.801 | 48.079 | -9.209  | 1.00 | 14.52 |
| ATOM | 2071 | CE1 | HIS | 259 | 22.701 | 49.050 | -9.270  | 1.00 | 12.90 |
| ATOM | 2072 | NE2 | HIS | 259 | 22.106 | 50.209 | -9.115  | 1.00 | 14.66 |
| ATOM | 2073 | C   | HIS | 259 | 18.949 | 47.746 | -11.296 | 1.00 | 9.17  |
| ATOM | 2074 | O   | HIS | 259 | 19.275 | 48.580 | -12.144 | 1.00 | 11.20 |
| ATOM | 2075 | N   | LEU | 260 | 19.091 | 46.450 | -11.529 | 1.00 | 9.71  |
| ATOM | 2076 | CA  | LEU | 260 | 19.763 | 45.917 | -12.699 | 1.00 | 11.16 |
| ATOM | 2077 | CB  | LEU | 260 | 19.771 | 44.362 | -12.647 | 1.00 | 13.64 |
| ATOM | 2078 | CG  | LEU | 260 | 20.621 | 43.697 | -11.579 | 1.00 | 14.53 |
| ATOM | 2079 | CD1 | LEU | 260 | 20.446 | 42.195 | -11.659 | 1.00 | 15.33 |
| ATOM | 2080 | CD2 | LEU | 260 | 22.081 | 44.131 | -11.700 | 1.00 | 18.49 |
| ATOM | 2081 | C   | LEU | 260 | 19.044 | 46.315 | -13.989 | 1.00 | 10.90 |
| ATOM | 2082 | O   | LEU | 260 | 19.715 | 46.435 | -15.017 | 1.00 | 11.94 |
| ATOM | 2083 | N   | THR | 261 | 17.723 | 46.442 | -13.932 | 1.00 | 9.82  |
| ATOM | 2084 | CA  | THR | 261 | 16.920 | 46.680 | -15.141 | 1.00 | 10.23 |
| ATOM | 2085 | CB  | THR | 261 | 15.671 | 45.798 | -15.202 | 1.00 | 9.32  |
| ATOM | 2086 | OG1 | THR | 261 | 14.737 | 46.138 | -14.174 | 1.00 | 9.59  |
| ATOM | 2087 | CG2 | THR | 261 | 16.000 | 44.325 | -15.098 | 1.00 | 10.96 |
| ATOM | 2088 | C   | THR | 261 | 16.492 | 48.151 | -15.298 | 1.00 | 10.83 |
| ATOM | 2089 | O   | THR | 261 | 15.664 | 48.493 | -16.138 | 1.00 | 12.22 |
| ATOM | 2090 | N   | ASN | 262 | 17.009 | 48.999 | -14.417 | 1.00 | 12.86 |
| ATOM | 2091 | CA  | ASN | 262 | 16.643 | 50.411 | -14.405 | 1.00 | 13.99 |
| ATOM | 2092 | CB  | ASN | 262 | 17.162 | 51.124 | -15.670 | 1.00 | 16.72 |
| ATOM | 2093 | CG  | ASN | 262 | 17.122 | 52.624 | -15.414 | 1.00 | 18.91 |
| ATOM | 2094 | OD1 | ASN | 262 | 17.484 | 53.032 | -14.306 | 1.00 | 23.20 |
| ATOM | 2095 | ND2 | ASN | 262 | 16.604 | 53.423 | -16.351 | 1.00 | 23.32 |
| ATOM | 2096 | C   | ASN | 262 | 15.143 | 50.639 | -14.281 | 1.00 | 14.56 |
| ATOM | 2097 | O   | ASN | 262 | 14.524 | 51.455 | -14.945 | 1.00 | 17.11 |
| ATOM | 2098 | N   | ASN | 263 | 14.570 | 49.836 | -13.381 | 1.00 | 13.82 |
| ATOM | 2099 | CA  | ASN | 263 | 13.148 | 49.902 | -13.081 | 1.00 | 15.46 |
| ATOM | 2100 | CB  | ASN | 263 | 12.863 | 51.289 | -12.502 | 1.00 | 17.97 |
| ATOM | 2101 | CG  | ASN | 263 | 12.214 | 51.276 | -11.157 | 1.00 | 17.06 |
| ATOM | 2102 | OD1 | ASN | 263 | 12.128 | 50.271 | -10.466 | 1.00 | 15.00 |
| ATOM | 2103 | ND2 | ASN | 263 | 11.533 | 52.359 | -10.866 | 1.00 | 25.64 |
| ATOM | 2104 | C   | ASN | 263 | 12.252 | 49.450 | -14.215 | 1.00 | 13.77 |
| ATOM | 2105 | O   | ASN | 263 | 11.012 | 49.566 | -14.160 | 1.00 | 18.41 |
| ATOM | 2106 | N   | TYR | 264 | 12.774 | 48.764 | -15.236 | 1.00 | 13.79 |
| ATOM | 2107 | CA  | TYR | 264 | 11.900 | 48.149 | -16.255 | 1.00 | 14.19 |
| ATOM | 2108 | CB  | TYR | 264 | 12.715 | 47.613 | -17.416 | 1.00 | 15.13 |
| ATOM | 2109 | CG  | TYR | 264 | 11.996 | 46.818 | -18.494 | 1.00 | 16.36 |
| ATOM | 2110 | CD1 | TYR | 264 | 11.035 | 47.371 | -19.362 | 1.00 | 17.78 |
| ATOM | 2111 | CE1 | TYR | 264 | 10.400 | 46.634 | -20.350 | 1.00 | 18.06 |
| ATOM | 2112 | CD2 | TYR | 264 | 12.259 | 45.484 | -18.745 | 1.00 | 16.68 |
| ATOM | 2113 | CE2 | TYR | 264 | 11.650 | 44.748 | -19.760 | 1.00 | 16.65 |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2114 | CZ  | TYR | 264 | 10.716 | 45.314 | -20.586 | 1.00 | 18.96 |
| ATOM | 2115 | OH  | TYR | 264 | 10.037 | 44.587 | -21.573 | 1.00 | 18.75 |
| ATOM | 2116 | C   | TYR | 264 | 11.078 | 47.051 | -15.593 | 1.00 | 12.40 |
| ATOM | 2117 | O   | TYR | 264 | 9.880  | 46.958 | -15.851 | 1.00 | 13.61 |
| ATOM | 2118 | N   | TYR | 265 | 11.724 | 46.245 | -14.738 | 1.00 | 10.62 |
| ATOM | 2119 | CA  | TYR | 265 | 11.038 | 45.308 | -13.845 | 1.00 | 9.32  |
| ATOM | 2120 | CB  | TYR | 265 | 11.580 | 43.896 | -13.877 | 1.00 | 9.65  |
| ATOM | 2121 | CG  | TYR | 265 | 11.384 | 43.145 | -15.197 | 1.00 | 9.18  |
| ATOM | 2122 | CD1 | TYR | 265 | 11.979 | 41.897 | -15.374 | 1.00 | 9.12  |
| ATOM | 2123 | CE1 | TYR | 265 | 11.788 | 41.151 | -16.513 | 1.00 | 9.35  |
| ATOM | 2124 | CD2 | TYR | 265 | 10.575 | 43.607 | -16.232 | 1.00 | 9.97  |
| ATOM | 2125 | CE2 | TYR | 265 | 10.412 | 42.861 | -17.391 | 1.00 | 9.60  |
| ATOM | 2126 | CZ  | TYR | 265 | 11.019 | 41.653 | -17.546 | 1.00 | 8.98  |
| ATOM | 2127 | OH  | TYR | 265 | 10.956 | 40.929 | -18.694 | 1.00 | 9.24  |
| ATOM | 2128 | C   | TYR | 265 | 11.143 | 45.898 | -12.455 | 1.00 | 8.87  |
| ATOM | 2129 | O   | TYR | 265 | 12.165 | 45.736 | -11.793 | 1.00 | 10.25 |
| ATOM | 2130 | N   | LYS | 266 | 10.091 | 46.591 | -12.039 | 1.00 | 9.35  |
| ATOM | 2131 | CA  | LYS | 266 | 10.042 | 47.206 | -10.722 | 1.00 | 10.27 |
| ATOM | 2132 | CB  | LYS | 266 | 8.764  | 48.067 | -10.642 | 1.00 | 11.78 |
| ATOM | 2133 | CG  | LYS | 266 | 8.798  | 49.269 | -11.544 | 1.00 | 15.74 |
| ATOM | 2134 | CD  | LYS | 266 | 7.679  | 50.219 | -11.609 | 1.00 | 20.41 |
| ATOM | 2135 | CE  | LYS | 266 | 8.060  | 51.436 | -12.461 | 1.00 | 27.15 |
| ATOM | 2136 | NZ  | LYS | 266 | 8.880  | 51.073 | -13.684 | 1.00 | 38.27 |
| ATOM | 2137 | C   | LYS | 266 | 9.917  | 46.141 | -9.642  | 1.00 | 9.64  |
| ATOM | 2138 | O   | LYS | 266 | 9.483  | 45.006 | -9.859  | 1.00 | 11.33 |
| ATOM | 2139 | N   | ALA | 267 | 10.398 | 46.485 | -8.457  | 1.00 | 8.21  |
| ATOM | 2140 | CA  | ALA | 267 | 10.177 | 45.669 | -7.302  | 1.00 | 8.00  |
| ATOM | 2141 | CB  | ALA | 267 | 11.263 | 45.935 | -6.279  | 1.00 | 9.27  |
| ATOM | 2142 | C   | ALA | 267 | 8.810  | 46.112 | -6.747  | 1.00 | 8.06  |
| ATOM | 2143 | O   | ALA | 267 | 8.703  | 47.252 | -6.265  | 1.00 | 9.31  |
| ATOM | 2144 | N   | PRO | 268 | 7.786  | 45.314 | -6.903  | 1.00 | 7.87  |
| ATOM | 2145 | CD  | PRO | 268 | 7.704  | 43.960 | -7.464  | 1.00 | 8.45  |
| ATOM | 2146 | CA  | PRO | 268 | 6.464  | 45.815 | -6.507  | 1.00 | 8.53  |
| ATOM | 2147 | CB  | PRO | 268 | 5.497  | 44.732 | -6.971  | 1.00 | 8.95  |
| ATOM | 2148 | CG  | PRO | 268 | 6.340  | 43.491 | -6.981  | 1.00 | 9.67  |
| ATOM | 2149 | C   | PRO | 268 | 6.342  | 46.060 | -5.020  | 1.00 | 7.51  |
| ATOM | 2150 | O   | PRO | 268 | 6.832  | 45.247 | -4.237  | 1.00 | 8.65  |
| ATOM | 2151 | N   | ILE | 269 | 5.648  | 47.157 | -4.658  | 1.00 | 7.63  |
| ATOM | 2152 | CA  | ILE | 269 | 5.356  | 47.441 | -3.254  | 1.00 | 7.94  |
| ATOM | 2153 | CB  | ILE | 269 | 5.120  | 48.928 | -2.981  | 1.00 | 9.79  |
| ATOM | 2154 | CG2 | ILE | 269 | 4.494  | 49.172 | -1.634  | 1.00 | 10.56 |
| ATOM | 2155 | CG1 | ILE | 269 | 6.437  | 49.720 | -3.185  | 1.00 | 13.68 |
| ATOM | 2156 | CD1 | ILE | 269 | 6.187  | 51.182 | -3.479  | 1.00 | 23.32 |
| ATOM | 2157 | C   | ILE | 269 | 4.170  | 46.593 | -2.837  | 1.00 | 7.83  |
| ATOM | 2158 | O   | ILE | 269 | 3.149  | 46.540 | -3.511  | 1.00 | 9.16  |
| ATOM | 2159 | N   | HIS | 270 | 4.317  | 45.894 | -1.703  | 1.00 | 7.29  |
| ATOM | 2160 | CA  | HIS | 270 | 3.276  | 45.019 | -1.206  | 1.00 | 7.01  |
| ATOM | 2161 | CB  | HIS | 270 | 3.400  | 43.626 | -1.835  | 1.00 | 7.25  |
| ATOM | 2162 | CG  | HIS | 270 | 4.744  | 43.024 | -1.598  | 1.00 | 7.13  |
| ATOM | 2163 | CD2 | HIS | 270 | 5.128  | 42.038 | -0.746  | 1.00 | 7.31  |
| ATOM | 2164 | ND1 | HIS | 270 | 5.880  | 43.389 | -2.273  | 1.00 | 7.07  |
| ATOM | 2165 | CE1 | HIS | 270 | 6.904  | 42.683 | -1.826  | 1.00 | 7.87  |
| ATOM | 2166 | NE2 | HIS | 270 | 6.489  | 41.831 | -0.890  | 1.00 | 7.31  |
| ATOM | 2167 | C   | HIS | 270 | 3.274  | 44.991 | 0.302   | 1.00 | 6.54  |
| ATOM | 2168 | O   | HIS | 270 | 4.212  | 45.458 | 0.936   | 1.00 | 7.63  |
| ATOM | 2169 | N   | ARG | 271 | 2.201  | 44.490 | 0.896   | 1.00 | 6.78  |
| ATOM | 2170 | CA  | ARG | 271 | 1.988  | 44.467 | 2.318   | 1.00 | 6.60  |
| ATOM | 2171 | CB  | ARG | 271 | 1.366  | 45.769 | 2.853   | 1.00 | 7.26  |
| ATOM | 2172 | CG  | ARG | 271 | -0.088 | 45.972 | 2.398   | 1.00 | 8.12  |
| ATOM | 2173 | CD  | ARG | 271 | -0.543 | 47.381 | 2.652   | 1.00 | 8.48  |
| ATOM | 2174 | NE  | ARG | 271 | -1.974 | 47.504 | 2.297   | 1.00 | 9.27  |
| ATOM | 2175 | CZ  | ARG | 271 | -2.643 | 48.651 | 2.312   | 1.00 | 9.64  |
| ATOM | 2176 | NH1 | ARG | 271 | -2.060 | 49.802 | 2.648   | 1.00 | 10.45 |
| ATOM | 2177 | NH2 | ARG | 271 | -3.930 | 48.660 | 1.968   | 1.00 | 11.63 |
| ATOM | 2178 | C   | ARG | 271 | 1.144  | 43.252 | 2.682   | 1.00 | 6.79  |
| ATOM | 2179 | O   | ARG | 271 | 0.517  | 42.637 | 1.805   | 1.00 | 7.95  |
| ATOM | 2180 | N   | VAL | 272 | 1.154  | 42.887 | 3.953   | 1.00 | 7.39  |
| ATOM | 2181 | CA  | VAL | 272 | 0.444  | 41.736 | 4.493   | 1.00 | 6.97  |
| ATOM | 2182 | CB  | VAL | 272 | 1.369  | 40.830 | 5.328   | 1.00 | 7.37  |
| ATOM | 2183 | CG1 | VAL | 272 | 0.615  | 39.661 | 5.865   | 1.00 | 9.31  |
| ATOM | 2184 | CG2 | VAL | 272 | 2.609  | 40.388 | 4.562   | 1.00 | 9.68  |
| ATOM | 2185 | C   | VAL | 272 | -0.712 | 42.173 | 5.378   | 1.00 | 6.78  |
| ATOM | 2186 | O   | VAL | 272 | -0.470 | 42.805 | 6.415   | 1.00 | 7.67  |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2187 | N   | LYS | 273 | -1.917 | 41.839 | 4.950  | 1.00 | 7.33  |
| ATOM | 2188 | CA  | LYS | 273 | -3.051 | 42.135 | 5.792  | 1.00 | 8.38  |
| ATOM | 2189 | CB  | LYS | 273 | -4.364 | 41.763 | 5.047  | 1.00 | 9.72  |
| ATOM | 2190 | CG  | LYS | 273 | -4.658 | 42.765 | 3.950  | 1.00 | 13.66 |
| ATOM | 2191 | CD  | LYS | 273 | -6.090 | 42.725 | 3.437  | 1.00 | 20.08 |
| ATOM | 2192 | CE  | LYS | 273 | -6.381 | 41.379 | 2.873  | 1.00 | 21.66 |
| ATOM | 2193 | NZ  | LYS | 273 | -7.801 | 41.227 | 2.413  | 1.00 | 19.22 |
| ATOM | 2194 | C   | LYS | 273 | -3.047 | 41.256 | 7.047  | 1.00 | 7.72  |
| ATOM | 2195 | O   | LYS | 273 | -2.628 | 40.112 | 7.023  | 1.00 | 8.06  |
| ATOM | 2196 | N   | TRP | 274 | -3.644 | 41.812 | 8.114  | 1.00 | 7.85  |
| ATOM | 2197 | CA  | TRP | 274 | -3.914 | 41.041 | 9.322  | 1.00 | 8.01  |
| ATOM | 2198 | CB  | TRP | 274 | -4.314 | 41.953 | 10.481 | 1.00 | 8.38  |
| ATOM | 2199 | CG  | TRP | 274 | -4.864 | 41.210 | 11.655 | 1.00 | 8.22  |
| ATOM | 2200 | CD2 | TRP | 274 | -6.226 | 41.225 | 12.078 | 1.00 | 8.59  |
| ATOM | 2201 | CE2 | TRP | 274 | -6.311 | 40.370 | 13.188 | 1.00 | 9.28  |
| ATOM | 2202 | CE3 | TRP | 274 | -7.393 | 41.859 | 11.630 | 1.00 | 10.81 |
| ATOM | 2203 | CD1 | TRP | 274 | -4.216 | 40.377 | 12.490 | 1.00 | 8.98  |
| ATOM | 2204 | NE1 | TRP | 274 | -5.074 | 39.850 | 13.430 | 1.00 | 9.16  |
| ATOM | 2205 | CZ2 | TRP | 274 | -7.485 | 40.145 | 13.881 | 1.00 | 9.84  |
| ATOM | 2206 | CZ3 | TRP | 274 | -8.570 | 41.630 | 12.309 | 1.00 | 12.76 |
| ATOM | 2207 | CH2 | TRP | 274 | -8.591 | 40.765 | 13.403 | 1.00 | 12.58 |
| ATOM | 2208 | C   | TRP | 274 | -5.114 | 40.123 | 9.043  | 1.00 | 7.32  |
| ATOM | 2209 | O   | TRP | 274 | -6.156 | 40.621 | 8.598  | 1.00 | 8.37  |
| ATOM | 2210 | N   | VAL | 275 | -4.963 | 38.854 | 9.345  | 1.00 | 7.40  |
| ATOM | 2211 | CA  | VAL | 275 | -6.042 | 37.883 | 9.221  | 1.00 | 7.99  |
| ATOM | 2212 | CB  | VAL | 275 | -5.913 | 37.057 | 7.931  | 1.00 | 11.04 |
| ATOM | 2213 | CG1 | VAL | 275 | -7.152 | 36.169 | 7.828  | 1.00 | 13.41 |
| ATOM | 2214 | CG2 | VAL | 275 | -5.765 | 37.904 | 6.702  | 1.00 | 15.17 |
| ATOM | 2215 | C   | VAL | 275 | -5.933 | 37.000 | 10.457 | 1.00 | 7.32  |
| ATOM | 2216 | O   | VAL | 275 | -4.818 | 36.547 | 10.759 | 1.00 | 8.66  |
| ATOM | 2217 | N   | ASN | 276 | -7.013 | 36.774 | 11.175 | 1.00 | 7.50  |
| ATOM | 2218 | CA  | ASN | 276 | -6.930 | 35.898 | 12.365 | 1.00 | 8.58  |
| ATOM | 2219 | CB  | ASN | 276 | -7.921 | 36.377 | 13.414 | 1.00 | 9.69  |
| ATOM | 2220 | CG  | ASN | 276 | -7.600 | 35.733 | 14.757 | 1.00 | 10.43 |
| ATOM | 2221 | OD1 | ASN | 276 | -6.631 | 34.956 | 14.885 | 1.00 | 12.06 |
| ATOM | 2222 | ND2 | ASN | 276 | -8.414 | 35.995 | 15.765 | 1.00 | 8.56  |
| ATOM | 2223 | C   | ASN | 276 | -7.172 | 34.443 | 11.976 | 1.00 | 9.02  |
| ATOM | 2224 | O   | ASN | 276 | -8.281 | 33.914 | 12.021 | 1.00 | 8.26  |
| ATOM | 2225 | N   | ALA | 277 | -6.107 | 33.815 | 11.504 | 1.00 | 8.04  |
| ATOM | 2226 | CA  | ALA | 277 | -6.107 | 32.466 | 10.982 | 1.00 | 9.72  |
| ATOM | 2227 | CB  | ALA | 277 | -6.438 | 32.469 | 9.514  | 1.00 | 7.91  |
| ATOM | 2228 | C   | ALA | 277 | -4.711 | 31.860 | 11.136 | 1.00 | 8.82  |
| ATOM | 2229 | O   | ALA | 277 | -3.705 | 32.537 | 10.998 | 1.00 | 7.51  |
| ATOM | 2230 | N   | GLU | 278 | -4.674 | 30.592 | 11.445 | 1.00 | 7.98  |
| ATOM | 2231 | CA  | GLU | 278 | -3.460 | 29.801 | 11.557 | 1.00 | 10.38 |
| ATOM | 2232 | CB  | GLU | 278 | -3.727 | 28.504 | 12.302 | 1.00 | 11.75 |
| ATOM | 2233 | CG  | GLU | 278 | -2.539 | 27.650 | 12.655 | 1.00 | 10.88 |
| ATOM | 2234 | CD  | GLU | 278 | -1.613 | 28.347 | 13.638 | 1.00 | 12.63 |
| ATOM | 2235 | OE1 | GLU | 278 | -0.419 | 28.424 | 13.314 | 1.00 | 10.57 |
| ATOM | 2236 | OE2 | GLU | 278 | -2.074 | 28.833 | 14.680 | 1.00 | 8.98  |
| ATOM | 2237 | C   | GLU | 278 | -3.034 | 29.524 | 10.111 | 1.00 | 12.15 |
| ATOM | 2238 | O   | GLU | 278 | -3.719 | 28.836 | 9.346  | 1.00 | 8.14  |
| ATOM | 2239 | N   | ARG | 279 | -1.864 | 30.037 | 9.738  | 1.00 | 8.39  |
| ATOM | 2240 | CA  | ARG | 279 | -1.410 | 29.901 | 8.373  | 1.00 | 10.37 |
| ATOM | 2241 | CB  | ARG | 279 | -2.095 | 30.906 | 7.472  | 1.00 | 10.01 |
| ATOM | 2242 | CG  | ARG | 279 | -1.659 | 32.310 | 7.818  | 1.00 | 9.69  |
| ATOM | 2243 | CD  | ARG | 279 | -2.541 | 33.367 | 7.101  | 1.00 | 9.29  |
| ATOM | 2244 | NE  | ARG | 279 | -2.026 | 34.712 | 7.405  | 1.00 | 9.20  |
| ATOM | 2245 | CZ  | ARG | 279 | -0.965 | 35.208 | 6.775  | 1.00 | 9.24  |
| ATOM | 2246 | NH1 | ARG | 279 | -0.368 | 34.596 | 5.774  | 1.00 | 9.29  |
| ATOM | 2247 | NH2 | ARG | 279 | -0.490 | 36.396 | 7.129  | 1.00 | 7.13  |
| ATOM | 2248 | C   | ARG | 279 | 0.095  | 29.920 | 8.275  | 1.00 | 8.10  |
| ATOM | 2249 | O   | ARG | 279 | 0.821  | 30.149 | 9.252  | 1.00 | 7.21  |
| ATOM | 2250 | N   | GLN | 280 | 0.593  | 29.601 | 7.095  | 1.00 | 7.07  |
| ATOM | 2251 | CA  | GLN | 280 | 2.006  | 29.505 | 6.778  | 1.00 | 8.87  |
| ATOM | 2252 | CB  | GLN | 280 | 2.318  | 28.088 | 6.255  | 1.00 | 8.89  |
| ATOM | 2253 | CG  | GLN | 280 | 2.043  | 27.047 | 7.312  | 1.00 | 8.58  |
| ATOM | 2254 | CD  | GLN | 280 | 2.188  | 25.645 | 6.771  | 1.00 | 11.01 |
| ATOM | 2255 | OE1 | GLN | 280 | 2.067  | 25.442 | 5.571  | 1.00 | 8.97  |
| ATOM | 2256 | NE2 | GLN | 280 | 2.533  | 24.689 | 7.591  | 1.00 | 6.21  |
| ATOM | 2257 | C   | GLN | 280 | 2.389  | 30.454 | 5.653  | 1.00 | 7.53  |
| ATOM | 2258 | O   | GLN | 280 | 1.634  | 30.606 | 4.671  | 1.00 | 6.11  |
| ATOM | 2259 | N   | SER | 281 | 3.554  | 31.037 | 5.779  | 1.00 |       |

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2260 | CA  | SER | 281 | 4.156  | 31.865 | 4.744  | 1.00 | 6.44  |
| ATOM | 2261 | CB  | SER | 281 | 4.016  | 33.345 | 5.109  | 1.00 | 7.40  |
| ATOM | 2262 | OG  | SER | 281 | 4.520  | 34.121 | 4.016  | 1.00 | 8.04  |
| ATOM | 2263 | C   | SER | 281 | 5.617  | 31.443 | 4.606  | 1.00 | 6.56  |
| ATOM | 2264 | O   | SER | 281 | 6.374  | 31.574 | 5.574  | 1.00 | 6.58  |
| ATOM | 2265 | N   | LEU | 282 | 5.952  | 30.778 | 3.493  | 1.00 | 5.40  |
| ATOM | 2266 | CA  | LEU | 282 | 7.243  | 30.105 | 3.352  | 1.00 | 6.03  |
| ATOM | 2267 | CB  | LEU | 282 | 6.986  | 28.583 | 3.195  | 1.00 | 6.16  |
| ATOM | 2268 | CG  | LEU | 282 | 5.982  | 27.942 | 4.203  | 1.00 | 7.21  |
| ATOM | 2269 | CD1 | LEU | 282 | 5.851  | 26.441 | 3.942  | 1.00 | 8.79  |
| ATOM | 2270 | CD2 | LEU | 282 | 6.340  | 28.188 | 5.661  | 1.00 | 8.29  |
| ATOM | 2271 | C   | LEU | 282 | 8.025  | 30.641 | 2.173  | 1.00 | 5.52  |
| ATOM | 2272 | O   | LEU | 282 | 8.055  | 30.039 | 1.071  | 1.00 | 5.66  |
| ATOM | 2273 | N   | PRO | 283 | 8.632  | 31.801 | 2.318  | 1.00 | 5.55  |
| ATOM | 2274 | CD  | PRO | 283 | 8.549  | 32.739 | 3.463  | 1.00 | 5.92  |
| ATOM | 2275 | CA  | PRO | 283 | 9.437  | 32.349 | 1.222  | 1.00 | 5.72  |
| ATOM | 2276 | CB  | PRO | 283 | 9.634  | 33.815 | 1.631  | 1.00 | 6.44  |
| ATOM | 2277 | CG  | PRO | 283 | 9.624  | 33.748 | 3.131  | 1.00 | 6.28  |
| ATOM | 2278 | C   | PRO | 283 | 10.795 | 31.729 | 1.057  | 1.00 | 4.97  |
| ATOM | 2279 | O   | PRO | 283 | 11.445 | 31.312 | 2.006  | 1.00 | 5.92  |
| ATOM | 2280 | N   | PHE | 284 | 11.262 | 31.720 | -0.187 | 1.00 | 5.22  |
| ATOM | 2281 | CA  | PHE | 284 | 12.642 | 31.498 | -0.602 | 1.00 | 4.80  |
| ATOM | 2282 | CB  | PHE | 284 | 12.785 | 30.323 | -1.566 | 1.00 | 5.14  |
| ATOM | 2283 | CG  | PHE | 284 | 14.184 | 29.960 | -1.983 | 1.00 | 4.79  |
| ATOM | 2284 | CD1 | PHE | 284 | 15.089 | 29.473 | -1.057 | 1.00 | 5.39  |
| ATOM | 2285 | CD2 | PHE | 284 | 14.591 | 30.026 | -3.286 | 1.00 | 5.88  |
| ATOM | 2286 | CE1 | PHE | 284 | 16.341 | 29.032 | -1.451 | 1.00 | 5.76  |
| ATOM | 2287 | CE2 | PHE | 284 | 15.828 | 29.633 | -3.714 | 1.00 | 5.70  |
| ATOM | 2288 | CZ  | PHE | 284 | 16.714 | 29.109 | -2.787 | 1.00 | 5.57  |
| ATOM | 2289 | C   | PHE | 284 | 13.119 | 32.795 | -1.263 | 1.00 | 4.78  |
| ATOM | 2290 | O   | PHE | 284 | 12.566 | 33.190 | -2.308 | 1.00 | 5.98  |
| ATOM | 2291 | N   | PHE | 285 | 14.114 | 33.448 | -0.659 | 1.00 | 5.01  |
| ATOM | 2292 | CA  | PHE | 285 | 14.656 | 34.687 | -1.215 | 1.00 | 5.10  |
| ATOM | 2293 | CB  | PHE | 285 | 15.058 | 35.637 | -0.062 | 1.00 | 6.13  |
| ATOM | 2294 | CG  | PHE | 285 | 13.858 | 36.096 | 0.747  | 1.00 | 6.38  |
| ATOM | 2295 | CD1 | PHE | 285 | 13.665 | 35.656 | 2.044  | 1.00 | 6.54  |
| ATOM | 2296 | CD2 | PHE | 285 | 12.909 | 36.933 | 0.195  | 1.00 | 6.45  |
| ATOM | 2297 | CE1 | PHE | 285 | 12.534 | 36.014 | 2.765  | 1.00 | 7.21  |
| ATOM | 2298 | CB2 | PHE | 285 | 11.781 | 37.303 | 0.891  | 1.00 | 7.45  |
| ATOM | 2299 | CZ  | PHE | 285 | 11.610 | 36.853 | 2.177  | 1.00 | 7.71  |
| ATOM | 2300 | C   | PHE | 285 | 15.812 | 34.333 | -2.108 | 1.00 | 5.08  |
| ATOM | 2301 | O   | PHE | 285 | 16.815 | 33.800 | -1.608 | 1.00 | 6.02  |
| ATOM | 2302 | N   | VAL | 286 | 15.658 | 34.588 | -3.399 | 1.00 | 5.58  |
| ATOM | 2303 | CA  | VAL | 286 | 16.696 | 34.255 | -4.364 | 1.00 | 5.96  |
| ATOM | 2304 | CB  | VAL | 286 | 16.104 | 34.056 | -5.766 | 1.00 | 5.78  |
| ATOM | 2305 | CG1 | VAL | 286 | 17.189 | 33.783 | -6.814 | 1.00 | 7.42  |
| ATOM | 2306 | CG2 | VAL | 286 | 15.065 | 32.922 | -5.710 | 1.00 | 7.19  |
| ATOM | 2307 | C   | VAL | 286 | 17.756 | 35.372 | -4.347 | 1.00 | 5.98  |
| ATOM | 2308 | O   | VAL | 286 | 17.569 | 36.453 | -4.895 | 1.00 | 6.92  |
| ATOM | 2309 | N   | ASN | 287 | 18.839 | 35.082 | -3.642 | 1.00 | 5.82  |
| ATOM | 2310 | CA  | ASN | 287 | 20.008 | 35.922 | -3.466 | 1.00 | 6.12  |
| ATOM | 2311 | CB  | ASN | 287 | 20.324 | 36.042 | -1.971 | 1.00 | 6.40  |
| ATOM | 2312 | CG  | ASN | 287 | 19.235 | 36.737 | -1.183 | 1.00 | 6.67  |
| ATOM | 2313 | OD1 | ASN | 287 | 18.623 | 37.682 | -1.683 | 1.00 | 7.35  |
| ATOM | 2314 | ND2 | ASN | 287 | 19.036 | 36.262 | 0.073  | 1.00 | 6.70  |
| ATOM | 2315 | C   | ASN | 287 | 21.187 | 35.296 | -4.216 | 1.00 | 5.72  |
| ATOM | 2316 | O   | ASN | 287 | 21.271 | 34.072 | -4.300 | 1.00 | 6.46  |
| ATOM | 2317 | N   | LEU | 288 | 22.049 | 36.145 | -4.781 | 1.00 | 6.71  |
| ATOM | 2318 | CA  | LEU | 288 | 23.223 | 35.679 | -5.499 | 1.00 | 6.46  |
| ATOM | 2319 | CB  | LEU | 288 | 23.538 | 36.703 | -6.595 | 1.00 | 7.57  |
| ATOM | 2320 | CG  | LEU | 288 | 22.371 | 36.977 | -7.570 | 1.00 | 8.20  |
| ATOM | 2321 | CD1 | LEU | 288 | 22.819 | 37.998 | -8.621 | 1.00 | 10.08 |
| ATOM | 2322 | CD2 | LEU | 288 | 21.880 | 35.687 | -8.189 | 1.00 | 8.32  |
| ATOM | 2323 | C   | LEU | 288 | 24.381 | 35.444 | -4.525 | 1.00 | 7.33  |
| ATOM | 2324 | O   | LEU | 288 | 24.140 | 35.277 | -3.317 | 1.00 | 8.58  |
| ATOM | 2325 | N   | GLY | 289 | 25.607 | 35.358 | -5.037 | 1.00 | 7.93  |
| ATOM | 2326 | CA  | GLY | 289 | 26.765 | 35.216 | -4.155 | 1.00 | 7.86  |
| ATOM | 2327 | C   | GLY | 289 | 27.242 | 36.571 | -3.667 | 1.00 | 7.24  |
| ATOM | 2328 | O   | GLY | 289 | 26.890 | 37.634 | -4.186 | 1.00 | 8.44  |
| ATOM | 2329 | N   | TYR | 290 | 28.075 | 36.559 | -2.633 | 1.00 | 7.71  |
| ATOM | 2330 | CA  | TYR | 290 | 28.503 | 37.789 | -1.986 | 1.00 | 8.91  |
| ATOM | 2331 | CB  | TYR | 290 | 29.407 | 37.453 | -0.813 | 1.00 | 9.56  |
| ATOM | 2332 | CG  | TYR | 290 | 29.638 | 38.614 | 0.135  | 1.00 | 9.12  |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2333 | CD1 | TYR | 290 | 28.720 | 38.961 | 1.118   | 1.00 | 10.55 |
| ATOM | 2334 | CE1 | TYR | 290 | 28.949 | 40.041 | 1.966   | 1.00 | 12.13 |
| ATOM | 2335 | CD2 | TYR | 290 | 30.792 | 39.367 | 0.036   | 1.00 | 12.09 |
| ATOM | 2336 | CE2 | TYR | 290 | 31.035 | 40.426 | 0.887   | 1.00 | 13.43 |
| ATOM | 2337 | CZ  | TYR | 290 | 30.129 | 40.766 | 1.861   | 1.00 | 13.85 |
| ATOM | 2338 | OH  | TYR | 290 | 30.407 | 41.847 | 2.679   | 1.00 | 16.61 |
| ATOM | 2339 | C   | TYR | 290 | 29.196 | 38.783 | -2.903  | 1.00 | 8.98  |
| ATOM | 2340 | O   | TYR | 290 | 28.979 | 39.980 | -2.814  | 1.00 | 9.66  |
| ATOM | 2341 | N   | ASP | 291 | 30.009 | 38.246 | -3.816  | 1.00 | 9.63  |
| ATOM | 2342 | CA  | ASP | 291 | 30.738 | 39.081 | -4.766  | 1.00 | 11.13 |
| ATOM | 2343 | CB  | ASP | 291 | 32.143 | 38.545 | -4.920  | 1.00 | 14.78 |
| ATOM | 2344 | CG  | ASP | 291 | 33.015 | 38.830 | -3.715  | 1.00 | 19.43 |
| ATOM | 2345 | OD1 | ASP | 291 | 34.005 | 38.109 | -3.515  | 1.00 | 30.38 |
| ATOM | 2346 | OD2 | ASP | 291 | 32.776 | 39.787 | -2.963  | 1.00 | 21.52 |
| ATOM | 2347 | C   | ASP | 291 | 30.075 | 39.198 | -6.123  | 1.00 | 10.76 |
| ATOM | 2348 | O   | ASP | 291 | 30.676 | 39.770 | -7.035  | 1.00 | 14.21 |
| ATOM | 2349 | N   | SER | 292 | 28.867 | 38.636 | -6.294  | 1.00 | 10.05 |
| ATOM | 2350 | CA  | SER | 292 | 28.226 | 38.714 | -7.606  | 1.00 | 9.39  |
| ATOM | 2351 | CB  | SER | 292 | 26.908 | 37.921 | -7.562  | 1.00 | 9.60  |
| ATOM | 2352 | OG  | SER | 292 | 27.117 | 36.538 | -7.241  | 1.00 | 10.02 |
| ATOM | 2353 | C   | SER | 292 | 27.915 | 40.181 | -7.922  | 1.00 | 9.65  |
| ATOM | 2354 | O   | SER | 292 | 27.303 | 40.934 | -7.170  | 1.00 | 10.11 |
| ATOM | 2355 | N   | VAL | 293 | 28.284 | 40.587 | -9.123  | 1.00 | 11.44 |
| ATOM | 2356 | CA  | VAL | 293 | 27.948 | 41.879 | -9.675  | 1.00 | 12.30 |
| ATOM | 2357 | CB  | VAL | 293 | 29.177 | 42.809 | -9.749  | 1.00 | 14.95 |
| ATOM | 2358 | CG1 | VAL | 293 | 28.691 | 44.199 | -10.166 | 1.00 | 20.38 |
| ATOM | 2359 | CG2 | VAL | 293 | 29.947 | 42.902 | -8.464  | 1.00 | 18.62 |
| ATOM | 2360 | C   | VAL | 293 | 27.402 | 41.683 | -11.091 | 1.00 | 13.15 |
| ATOM | 2361 | O   | VAL | 293 | 27.976 | 41.020 | -11.971 | 1.00 | 17.31 |
| ATOM | 2362 | N   | ILE | 294 | 26.232 | 42.246 | -11.309 | 1.00 | 13.36 |
| ATOM | 2363 | CA  | ILE | 294 | 25.669 | 42.289 | -12.650 | 1.00 | 16.26 |
| ATOM | 2364 | CB  | ILE | 294 | 24.283 | 41.645 | -12.648 | 1.00 | 18.21 |
| ATOM | 2365 | CG2 | ILE | 294 | 23.540 | 41.879 | -13.941 | 1.00 | 22.79 |
| ATOM | 2366 | CG1 | ILE | 294 | 24.529 | 40.135 | -12.350 | 1.00 | 19.50 |
| ATOM | 2367 | CD1 | ILE | 294 | 23.255 | 39.371 | -12.397 | 1.00 | 21.00 |
| ATOM | 2368 | C   | ILE | 294 | 25.616 | 43.756 | -13.059 | 1.00 | 14.95 |
| ATOM | 2369 | O   | ILE | 294 | 25.193 | 44.619 | -12.311 | 1.00 | 14.96 |
| ATOM | 2370 | N   | ASP | 295 | 26.164 | 44.020 | -14.235 | 1.00 | 15.39 |
| ATOM | 2371 | CA  | ASP | 295 | 26.203 | 45.398 | -14.709 | 1.00 | 16.58 |
| ATOM | 2372 | CB  | ASP | 295 | 27.214 | 45.501 | -15.857 | 1.00 | 23.82 |
| ATOM | 2373 | CG  | ASP | 295 | 28.612 | 45.188 | -15.298 | 1.00 | 30.17 |
| ATOM | 2374 | OD1 | ASP | 295 | 29.304 | 44.457 | -16.044 | 1.00 | 42.83 |
| ATOM | 2375 | OD2 | ASP | 295 | 29.000 | 45.638 | -14.184 | 1.00 | 32.91 |
| ATOM | 2376 | C   | ASP | 295 | 24.803 | 45.841 | -15.109 | 1.00 | 13.64 |
| ATOM | 2377 | O   | ASP | 295 | 24.072 | 45.199 | -15.856 | 1.00 | 14.07 |
| ATOM | 2378 | N   | PRO | 296 | 24.390 | 46.969 | -14.533 | 1.00 | 12.78 |
| ATOM | 2379 | CD  | PRO | 296 | 25.049 | 47.684 | -13.426 | 1.00 | 14.44 |
| ATOM | 2380 | CA  | PRO | 296 | 23.029 | 47.467 | -14.847 | 1.00 | 12.67 |
| ATOM | 2381 | CB  | PRO | 296 | 22.877 | 48.659 | -13.923 | 1.00 | 14.23 |
| ATOM | 2382 | CG  | PRO | 296 | 23.840 | 48.351 | -12.818 | 1.00 | 16.25 |
| ATOM | 2383 | C   | PRO | 296 | 22.825 | 47.803 | -16.319 | 1.00 | 12.63 |
| ATOM | 2384 | O   | PRO | 296 | 23.750 | 48.221 | -17.032 | 1.00 | 14.48 |
| ATOM | 2385 | N   | PHE | 297 | 21.602 | 47.615 | -16.800 | 1.00 | 11.48 |
| ATOM | 2386 | CA  | PHE | 297 | 21.260 | 47.872 | -18.195 | 1.00 | 11.96 |
| ATOM | 2387 | CB  | PHE | 297 | 21.388 | 46.632 | -19.046 | 1.00 | 12.04 |
| ATOM | 2388 | CG  | PHE | 297 | 20.543 | 45.425 | -18.690 | 1.00 | 12.30 |
| ATOM | 2389 | CD1 | PHE | 297 | 19.390 | 45.126 | -19.386 | 1.00 | 15.33 |
| ATOM | 2390 | CD2 | PHE | 297 | 20.900 | 44.597 | -17.664 | 1.00 | 12.58 |
| ATOM | 2391 | CE1 | PHE | 297 | 18.648 | 44.005 | -19.091 | 1.00 | 17.14 |
| ATOM | 2392 | CE2 | PHE | 297 | 20.121 | 43.510 | -17.311 | 1.00 | 14.52 |
| ATOM | 2393 | CZ  | PHE | 297 | 18.969 | 43.235 | -18.003 | 1.00 | 16.56 |
| ATOM | 2394 | C   | PHE | 297 | 19.837 | 48.421 | -18.246 | 1.00 | 13.07 |
| ATOM | 2395 | O   | PHE | 297 | 19.162 | 48.472 | -17.219 | 1.00 | 14.15 |
| ATOM | 2396 | N   | ASP | 298 | 19.390 | 48.809 | -19.429 | 1.00 | 16.06 |
| ATOM | 2397 | CA  | ASP | 298 | 18.024 | 49.272 | -19.601 | 1.00 | 15.45 |
| ATOM | 2398 | CB  | ASP | 298 | 18.023 | 50.788 | -19.547 | 1.00 | 17.44 |
| ATOM | 2399 | CG  | ASP | 298 | 16.619 | 51.374 | -19.488 | 1.00 | 17.86 |
| ATOM | 2400 | OD1 | ASP | 298 | 15.634 | 50.717 | -19.809 | 1.00 | 17.50 |
| ATOM | 2401 | OD2 | ASP | 298 | 16.580 | 52.580 | -19.143 | 1.00 | 20.86 |
| ATOM | 2402 | C   | ASP | 298 | 17.436 | 48.753 | -20.900 | 1.00 | 16.52 |
| ATOM | 2403 | O   | ASP | 298 | 17.736 | 49.281 | -21.973 | 1.00 | 17.05 |
| ATOM | 2404 | N   | PRO | 299 | 16.541 | 47.776 | -20.829 | 1.00 | 16.19 |
| ATOM | 2405 | CD  | PRO | 299 | 16.199 | 47.050 | -19.589 | 1.00 | 17.38 |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2406 | CA  | PRO | 299 | 15.887 | 47.212 | -22.014 | 1.00 | 16.63 |
| ATOM | 2407 | CB  | PRO | 299 | 15.397 | 45.853 | -21.561 | 1.00 | 19.69 |
| ATOM | 2408 | CG  | PRO | 299 | 15.676 | 45.745 | -20.112 | 1.00 | 21.06 |
| ATOM | 2409 | C   | PRO | 299 | 14.854 | 48.081 | -22.726 | 1.00 | 17.45 |
| ATOM | 2410 | O   | PRO | 299 | 14.213 | 47.662 | -23.730 | 1.00 | 18.54 |
| ATOM | 2411 | N   | ARG | 300 | 14.703 | 49.327 | -22.232 | 1.00 | 16.34 |
| ATOM | 2412 | CA  | ARG | 300 | 13.857 | 50.321 | -22.881 | 1.00 | 18.12 |
| ATOM | 2413 | CB  | ARG | 300 | 13.086 | 51.146 | -21.833 | 1.00 | 19.33 |
| ATOM | 2414 | CG  | ARG | 300 | 11.959 | 50.301 | -21.242 | 1.00 | 21.93 |
| ATOM | 2415 | CD  | ARG | 300 | 11.237 | 50.861 | -20.020 | 1.00 | 25.26 |
| ATOM | 2416 | NE  | ARG | 300 | 12.231 | 51.198 | -19.046 | 1.00 | 30.85 |
| ATOM | 2417 | CZ  | ARG | 300 | 12.419 | 51.701 | -17.857 | 1.00 | 29.50 |
| ATOM | 2418 | NH1 | ARG | 300 | 11.422 | 52.069 | -17.096 | 1.00 | 32.95 |
| ATOM | 2419 | NH2 | ARG | 300 | 13.671 | 51.781 | -17.407 | 1.00 | 30.69 |
| ATOM | 2420 | C   | ARG | 300 | 14.691 | 51.279 | -23.726 | 1.00 | 17.96 |
| ATOM | 2421 | O   | ARG | 300 | 14.138 | 52.081 | -24.462 | 1.00 | 17.01 |
| ATOM | 2422 | N   | GLU | 301 | 15.997 | 51.254 | -23.552 | 1.00 | 17.71 |
| ATOM | 2423 | CA  | GLU | 301 | 16.913 | 52.185 | -24.206 | 1.00 | 19.38 |
| ATOM | 2424 | C   | GLU | 301 | 17.619 | 51.524 | -25.392 | 1.00 | 18.52 |
| ATOM | 2425 | O   | GLU | 301 | 18.127 | 50.400 | -25.261 | 1.00 | 17.52 |
| ATOM | 2426 | CB  | GLU | 301 | 17.949 | 52.595 | -23.157 | 1.00 | 23.66 |
| ATOM | 2427 | CG  | GLU | 301 | 17.521 | 53.757 | -22.322 | 1.00 | 27.35 |
| ATOM | 2428 | CD  | GLU | 301 | 16.969 | 54.959 | -23.059 | 1.00 | 32.53 |
| ATOM | 2429 | OE1 | GLU | 301 | 17.705 | 55.499 | -23.901 | 1.00 | 38.75 |
| ATOM | 2430 | OE2 | GLU | 301 | 15.841 | 55.411 | -22.764 | 1.00 | 38.29 |
| ATOM | 2431 | N   | PRO | 302 | 17.667 | 52.160 | -26.553 | 1.00 | 18.63 |
| ATOM | 2432 | CD  | PRO | 302 | 17.042 | 53.464 | -26.839 | 1.00 | 21.36 |
| ATOM | 2433 | CA  | PRO | 302 | 18.277 | 51.571 | -27.738 | 1.00 | 20.96 |
| ATOM | 2434 | CB  | PRO | 302 | 18.222 | 52.693 | -28.776 | 1.00 | 22.61 |
| ATOM | 2435 | CG  | PRO | 302 | 17.001 | 53.446 | -28.341 | 1.00 | 22.90 |
| ATOM | 2436 | C   | PRO | 302 | 19.683 | 51.057 | -27.579 | 1.00 | 21.62 |
| ATOM | 2437 | O   | PRO | 302 | 19.874 | 49.926 | -28.009 | 1.00 | 24.93 |
| ATOM | 2438 | N   | ASN | 303 | 20.520 | 51.712 | -26.771 | 1.00 | 21.61 |
| ATOM | 2439 | CA  | ASN | 303 | 21.840 | 51.125 | -26.582 | 1.00 | 22.90 |
| ATOM | 2440 | CB  | ASN | 303 | 22.905 | 52.194 | -26.448 | 1.00 | 26.88 |
| ATOM | 2441 | CG  | ASN | 303 | 22.642 | 53.204 | -25.353 | 1.00 | 27.57 |
| ATOM | 2442 | OD1 | ASN | 303 | 21.822 | 52.996 | -24.467 | 1.00 | 23.80 |
| ATOM | 2443 | ND2 | ASN | 303 | 23.353 | 54.329 | -25.453 | 1.00 | 29.21 |
| ATOM | 2444 | C   | ASN | 303 | 21.931 | 50.221 | -25.360 | 1.00 | 20.67 |
| ATOM | 2445 | O   | ASN | 303 | 23.039 | 49.773 | -25.049 | 1.00 | 23.78 |
| ATOM | 2446 | N   | GLY | 304 | 20.847 | 49.989 | -24.661 | 1.00 | 17.93 |
| ATOM | 2447 | CA  | GLY | 304 | 20.793 | 49.190 | -23.443 | 1.00 | 18.03 |
| ATOM | 2448 | C   | GLY | 304 | 21.488 | 49.856 | -22.276 | 1.00 | 17.52 |
| ATOM | 2449 | O   | GLY | 304 | 21.576 | 49.239 | -21.215 | 1.00 | 20.50 |
| ATOM | 2450 | N   | LYS | 305 | 22.009 | 51.071 | -22.342 | 1.00 | 18.09 |
| ATOM | 2451 | CA  | LYS | 305 | 22.768 | 51.590 | -21.208 | 1.00 | 20.79 |
| ATOM | 2452 | C   | LYS | 305 | 21.921 | 52.252 | -20.147 | 1.00 | 20.39 |
| ATOM | 2453 | O   | LYS | 305 | 20.850 | 52.777 | -20.392 | 1.00 | 21.26 |
| ATOM | 2454 | CB  | LYS | 305 | 23.884 | 52.524 | -21.675 | 1.00 | 24.72 |
| ATOM | 2455 | CG  | LYS | 305 | 25.002 | 51.789 | -22.421 | 1.00 | 30.61 |
| ATOM | 2456 | CD  | LYS | 305 | 26.032 | 52.816 | -22.869 | 1.00 | 36.33 |
| ATOM | 2457 | CE  | LYS | 305 | 26.246 | 52.908 | -24.360 | 1.00 | 39.54 |
| ATOM | 2458 | NZ  | LYS | 305 | 27.649 | 52.574 | -24.760 | 1.00 | 51.21 |
| ATOM | 2459 | N   | SER | 306 | 22.461 | 52.202 | -18.921 | 1.00 | 18.96 |
| ATOM | 2460 | CA  | SER | 306 | 21.758 | 52.837 | -17.816 | 1.00 | 19.30 |
| ATOM | 2461 | CB  | SER | 306 | 21.210 | 51.732 | -16.911 | 1.00 | 23.77 |
| ATOM | 2462 | OG  | SER | 306 | 21.758 | 51.769 | -15.640 | 1.00 | 26.38 |
| ATOM | 2463 | C   | SER | 306 | 22.711 | 53.732 | -17.050 | 1.00 | 16.95 |
| ATOM | 2464 | O   | SER | 306 | 23.919 | 53.528 | -16.996 | 1.00 | 20.29 |
| ATOM | 2465 | N   | ASP | 307 | 22.159 | 54.728 | -16.365 | 1.00 | 18.07 |
| ATOM | 2466 | CA  | ASP | 307 | 22.902 | 55.647 | -15.527 | 1.00 | 17.75 |
| ATOM | 2467 | CB  | ASP | 307 | 22.343 | 57.066 | -15.646 | 1.00 | 19.69 |
| ATOM | 2468 | CG  | ASP | 307 | 22.554 | 57.644 | -17.030 | 1.00 | 21.31 |
| ATOM | 2469 | OD1 | ASP | 307 | 23.544 | 57.289 | -17.717 | 1.00 | 25.76 |
| ATOM | 2470 | OD2 | ASP | 307 | 21.697 | 58.413 | -17.492 | 1.00 | 22.42 |
| ATOM | 2471 | C   | ASP | 307 | 23.003 | 55.194 | -14.083 | 1.00 | 17.12 |
| ATOM | 2472 | O   | ASP | 307 | 23.267 | 55.998 | -13.150 | 1.00 | 15.97 |
| ATOM | 2473 | N   | ARG | 308 | 22.897 | 53.886 | -13.877 | 1.00 | 18.84 |
| ATOM | 2474 | CA  | ARG | 308 | 23.109 | 53.313 | -12.542 | 1.00 | 17.51 |
| ATOM | 2475 | CB  | ARG | 308 | 22.067 | 52.271 | -12.242 | 1.00 | 16.86 |
| ATOM | 2476 | CG  | ARG | 308 | 20.688 | 52.745 | -11.848 | 1.00 | 15.69 |
| ATOM | 2477 | CD  | ARG | 308 | 19.627 | 51.694 | -11.982 | 1.00 | 18.04 |
| ATOM | 2478 | NE  | ARG | 308 | 18.312 | 52.224 | -11.687 | 1.00 | 17.41 |

|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2479 | CZ  | ARG | 308 | 17.733 | 52.219 | -10.497 | 1.00 | 15.39 |
| ATOM | 2480 | NH1 | ARG | 308 | 18.288 | 51.740 | -9.404  | 1.00 | 14.58 |
| ATOM | 2481 | NH2 | ARG | 308 | 16.517 | 52.713 | -10.426 | 1.00 | 19.03 |
| ATOM | 2482 | C   | ARG | 308 | 24.511 | 52.680 | -12.443 | 1.00 | 18.59 |
| ATOM | 2483 | O   | ARG | 308 | 25.055 | 52.218 | -13.440 | 1.00 | 25.55 |
| ATOM | 2484 | N   | GLU | 309 | 25.070 | 52.659 | -11.241 | 1.00 | 18.16 |
| ATOM | 2485 | CA  | GLU | 309 | 26.350 | 52.054 | -10.946 | 1.00 | 19.38 |
| ATOM | 2486 | CB  | GLU | 309 | 27.058 | 52.935 | -9.907  | 1.00 | 21.98 |
| ATOM | 2487 | CG  | GLU | 309 | 27.442 | 54.299 | -10.501 | 1.00 | 25.52 |
| ATOM | 2488 | CD  | GLU | 309 | 28.319 | 54.244 | -11.731 | 1.00 | 30.05 |
| ATOM | 2489 | OE1 | GLU | 309 | 29.244 | 53.401 | -11.842 | 1.00 | 36.16 |
| ATOM | 2490 | OE2 | GLU | 309 | 28.114 | 55.058 | -12.663 | 1.00 | 37.66 |
| ATOM | 2491 | C   | GLU | 309 | 26.233 | 50.607 | -10.484 | 1.00 | 15.87 |
| ATOM | 2492 | O   | GLU | 309 | 25.287 | 50.180 | -9.826  | 1.00 | 14.89 |
| ATOM | 2493 | N   | PRO | 310 | 27.164 | 49.735 | -10.842 | 1.00 | 14.73 |
| ATOM | 2494 | CD  | PRO | 310 | 28.275 | 50.012 | -11.799 | 1.00 | 16.91 |
| ATOM | 2495 | CA  | PRO | 310 | 27.152 | 48.348 | -10.386 | 1.00 | 15.04 |
| ATOM | 2496 | CB  | PRO | 310 | 28.419 | 47.733 | -11.059 | 1.00 | 17.03 |
| ATOM | 2497 | CG  | PRO | 310 | 28.700 | 48.625 | -12.220 | 1.00 | 19.09 |
| ATOM | 2498 | C   | PRO | 310 | 27.219 | 48.266 | -8.874  | 1.00 | 13.88 |
| ATOM | 2499 | O   | PRO | 310 | 27.841 | 49.068 | -8.164  | 1.00 | 15.60 |
| ATOM | 2500 | N   | LEU | 311 | 26.474 | 47.318 | -8.360  | 1.00 | 12.14 |
| ATOM | 2501 | CA  | LEU | 311 | 26.338 | 47.085 | -6.922  | 1.00 | 11.25 |
| ATOM | 2502 | CB  | LEU | 311 | 24.878 | 47.460 | -6.615  | 1.00 | 13.56 |
| ATOM | 2503 | CG  | LEU | 311 | 24.457 | 47.333 | -5.180  | 1.00 | 13.90 |
| ATOM | 2504 | CD1 | LEU | 311 | 25.339 | 48.120 | -4.233  | 1.00 | 20.42 |
| ATOM | 2505 | CD2 | LEU | 311 | 22.986 | 47.700 | -5.047  | 1.00 | 17.32 |
| ATOM | 2506 | C   | LEU | 311 | 26.572 | 45.604 | -6.622  | 1.00 | 10.64 |
| ATOM | 2507 | O   | LEU | 311 | 25.915 | 44.759 | -7.247  | 1.00 | 11.74 |
| ATOM | 2508 | N   | SER | 312 | 27.494 | 45.257 | -5.728  | 1.00 | 10.37 |
| ATOM | 2509 | CA  | SER | 312 | 27.725 | 43.854 | -5.407  | 1.00 | 11.32 |
| ATOM | 2510 | CB  | SER | 312 | 29.040 | 43.653 | -4.645  | 1.00 | 13.83 |
| ATOM | 2511 | OG  | SER | 312 | 28.821 | 43.933 | -3.284  | 1.00 | 20.95 |
| ATOM | 2512 | C   | SER | 312 | 26.576 | 43.311 | -4.593  | 1.00 | 9.82  |
| ATOM | 2513 | O   | SER | 312 | 26.000 | 44.059 | -3.793  | 1.00 | 11.18 |
| ATOM | 2514 | N   | TYR | 313 | 26.260 | 42.025 | -4.815  | 1.00 | 9.06  |
| ATOM | 2515 | CA  | TYR | 313 | 25.095 | 41.471 | -4.152  | 1.00 | 8.56  |
| ATOM | 2516 | CB  | TYR | 313 | 24.722 | 40.082 | -4.734  | 1.00 | 9.03  |
| ATOM | 2517 | CG  | TYR | 313 | 23.265 | 39.812 | -4.375  | 1.00 | 7.11  |
| ATOM | 2518 | CD1 | TYR | 313 | 22.290 | 40.192 | -5.276  | 1.00 | 8.14  |
| ATOM | 2519 | CE1 | TYR | 313 | 20.951 | 40.004 | -5.038  | 1.00 | 8.04  |
| ATOM | 2520 | CD2 | TYR | 313 | 22.871 | 39.273 | -3.179  | 1.00 | 6.33  |
| ATOM | 2521 | CE2 | TYR | 313 | 21.525 | 39.151 | -2.889  | 1.00 | 6.78  |
| ATOM | 2522 | CZ  | TYR | 313 | 20.558 | 39.481 | -3.810  | 1.00 | 6.87  |
| ATOM | 2523 | OH  | TYR | 313 | 19.227 | 39.413 | -3.570  | 1.00 | 7.92  |
| ATOM | 2524 | C   | TYR | 313 | 25.247 | 41.465 | -2.642  | 1.00 | 8.88  |
| ATOM | 2525 | O   | TYR | 313 | 24.295 | 41.721 | -1.876  | 1.00 | 8.66  |
| ATOM | 2526 | N   | GLY | 314 | 26.436 | 41.154 | -2.137  | 1.00 | 9.27  |
| ATOM | 2527 | CA  | GLY | 314 | 26.636 | 41.130 | -0.699  | 1.00 | 10.93 |
| ATOM | 2528 | C   | GLY | 314 | 26.438 | 42.475 | -0.028  | 1.00 | 11.24 |
| ATOM | 2529 | O   | GLY | 314 | 25.837 | 42.532 | 1.044   | 1.00 | 11.92 |
| ATOM | 2530 | N   | ASP | 315 | 26.927 | 43.543 | -0.658  | 1.00 | 12.52 |
| ATOM | 2531 | CA  | ASP | 315 | 26.682 | 44.876 | -0.145  | 1.00 | 13.51 |
| ATOM | 2532 | C   | ASP | 315 | 25.178 | 45.169 | -0.126  | 1.00 | 11.36 |
| ATOM | 2533 | O   | ASP | 315 | 24.643 | 45.674 | 0.871   | 1.00 | 12.03 |
| ATOM | 2534 | CB  | ASP | 315 | 27.367 | 45.918 | -1.023  | 1.00 | 18.60 |
| ATOM | 2535 | CG  | ASP | 315 | 28.845 | 46.015 | -0.671  | 1.00 | 23.51 |
| ATOM | 2536 | OD1 | ASP | 315 | 29.308 | 45.275 | 0.214   | 1.00 | 34.09 |
| ATOM | 2537 | OD2 | ASP | 315 | 29.448 | 46.876 | -1.358  | 1.00 | 38.29 |
| ATOM | 2538 | N   | TYR | 316 | 24.538 | 44.902 | -1.265  | 1.00 | 10.83 |
| ATOM | 2539 | CA  | TYR | 316 | 23.095 | 45.065 | -1.383  | 1.00 | 9.46  |
| ATOM | 2540 | CB  | TYR | 316 | 22.621 | 44.578 | -2.740  | 1.00 | 9.26  |
| ATOM | 2541 | CG  | TYR | 316 | 21.130 | 44.397 | -2.840  | 1.00 | 8.60  |
| ATOM | 2542 | CD1 | TYR | 316 | 20.273 | 45.477 | -3.037  | 1.00 | 8.34  |
| ATOM | 2543 | CE1 | TYR | 316 | 18.913 | 45.293 | -3.143  | 1.00 | 7.74  |
| ATOM | 2544 | CD2 | TYR | 316 | 20.585 | 43.119 | -2.768  | 1.00 | 7.91  |
| ATOM | 2545 | CE2 | TYR | 316 | 19.210 | 42.953 | -2.847  | 1.00 | 7.88  |
| ATOM | 2546 | CZ  | TYR | 316 | 18.381 | 44.028 | -3.021  | 1.00 | 8.21  |
| ATOM | 2547 | OH  | TYR | 316 | 17.021 | 43.799 | -3.101  | 1.00 | 8.23  |
| ATOM | 2548 | C   | TYR | 316 | 22.328 | 44.386 | -0.260  | 1.00 | 8.68  |
| ATOM | 2549 | O   | TYR | 316 | 21.435 | 44.940 | 0.393   | 1.00 | 8.47  |
| ATOM | 2550 | N   | LEU | 317 | 22.637 | 43.104 | -0.045  | 1.00 | 8.58  |
| ATOM | 2551 | CA  | LEU | 317 | 21.902 | 42.282 | 0.915   | 1.00 |       |

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|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2552 | CB  | LEU | 317 | 22.285 | 40.787 | 0.743  | 1.00 | 8.79  |
| ATOM | 2553 | CG  | LEU | 317 | 21.561 | 39.779 | 1.629  | 1.00 | 8.20  |
| ATOM | 2554 | CD1 | LEU | 317 | 20.073 | 39.788 | 1.272  | 1.00 | 9.81  |
| ATOM | 2555 | CD2 | LEU | 317 | 22.141 | 38.375 | 1.492  | 1.00 | 10.08 |
| ATOM | 2556 | C   | LEU | 317 | 22.107 | 42.735 | 2.352  | 1.00 | 8.90  |
| ATOM | 2557 | O   | LEU | 317 | 21.144 | 42.841 | 3.087  | 1.00 | 9.53  |
| ATOM | 2558 | N   | GLN | 318 | 23.362 | 42.918 | 2.770  | 1.00 | 10.62 |
| ATOM | 2559 | CA  | GLN | 318 | 23.615 | 43.262 | 4.185  | 1.00 | 12.66 |
| ATOM | 2560 | CB  | GLN | 318 | 25.124 | 43.337 | 4.464  | 1.00 | 14.04 |
| ATOM | 2561 | CG  | GLN | 318 | 25.445 | 43.620 | 5.905  | 1.00 | 19.74 |
| ATOM | 2562 | CD  | GLN | 318 | 26.927 | 43.890 | 6.154  | 1.00 | 23.96 |
| ATOM | 2563 | OE1 | GLN | 318 | 27.714 | 44.211 | 5.249  | 1.00 | 35.18 |
| ATOM | 2564 | NE2 | GLN | 318 | 27.322 | 43.856 | 7.426  | 1.00 | 29.80 |
| ATOM | 2565 | C   | GLN | 318 | 22.915 | 44.561 | 4.553  | 1.00 | 12.86 |
| ATOM | 2566 | O   | GLN | 318 | 22.198 | 44.673 | 5.560  | 1.00 | 15.11 |
| ATOM | 2567 | N   | ASN | 319 | 23.013 | 45.524 | 3.641  | 1.00 | 12.55 |
| ATOM | 2568 | CA  | ASN | 319 | 22.346 | 46.806 | 3.917  | 1.00 | 14.03 |
| ATOM | 2569 | CB  | ASN | 319 | 23.012 | 47.860 | 3.043  | 1.00 | 20.38 |
| ATOM | 2570 | CG  | ASN | 319 | 24.469 | 48.100 | 3.472  | 1.00 | 27.04 |
| ATOM | 2571 | OD1 | ASN | 319 | 24.837 | 48.041 | 4.669  | 1.00 | 36.52 |
| ATOM | 2572 | ND2 | ASN | 319 | 25.310 | 48.297 | 2.465  | 1.00 | 38.86 |
| ATOM | 2573 | C   | ASN | 319 | 20.844 | 46.703 | 3.764  | 1.00 | 11.80 |
| ATOM | 2574 | O   | ASN | 319 | 20.143 | 47.296 | 4.593  | 1.00 | 11.96 |
| ATOM | 2575 | N   | GLY | 320 | 20.312 | 45.946 | 2.806  | 1.00 | 9.58  |
| ATOM | 2576 | CA  | GLY | 320 | 18.902 | 45.829 | 2.624  | 1.00 | 9.89  |
| ATOM | 2577 | C   | GLY | 320 | 18.179 | 45.194 | 3.797  | 1.00 | 9.39  |
| ATOM | 2578 | O   | GLY | 320 | 17.091 | 45.598 | 4.167  | 1.00 | 10.40 |
| ATOM | 2579 | N   | LEU | 321 | 18.797 | 44.151 | 4.363  | 1.00 | 9.14  |
| ATOM | 2580 | CA  | LEU | 321 | 18.153 | 43.464 | 5.485  | 1.00 | 9.96  |
| ATOM | 2581 | CB  | LEU | 321 | 18.857 | 42.133 | 5.768  | 1.00 | 10.64 |
| ATOM | 2582 | CG  | LEU | 321 | 18.723 | 41.078 | 4.638  | 1.00 | 10.47 |
| ATOM | 2583 | CD1 | LEU | 321 | 19.399 | 39.826 | 5.109  | 1.00 | 15.39 |
| ATOM | 2584 | CD2 | LEU | 321 | 17.262 | 40.824 | 4.233  | 1.00 | 12.12 |
| ATOM | 2585 | C   | LEU | 321 | 18.108 | 44.339 | 6.710  | 1.00 | 10.07 |
| ATOM | 2586 | O   | LEU | 321 | 17.089 | 44.340 | 7.437  | 1.00 | 10.21 |
| ATOM | 2587 | N   | VAL | 322 | 19.176 | 45.095 | 6.956  | 1.00 | 10.17 |
| ATOM | 2588 | CA  | VAL | 322 | 19.146 | 46.035 | 8.069  | 1.00 | 11.92 |
| ATOM | 2589 | CB  | VAL | 322 | 20.532 | 46.687 | 8.252  | 1.00 | 14.76 |
| ATOM | 2590 | CG1 | VAL | 322 | 20.397 | 47.770 | 9.346  | 1.00 | 20.10 |
| ATOM | 2591 | CG2 | VAL | 322 | 21.537 | 45.651 | 8.753  | 1.00 | 21.00 |
| ATOM | 2592 | C   | VAL | 322 | 18.095 | 47.100 | 7.854  | 1.00 | 10.68 |
| ATOM | 2593 | O   | VAL | 322 | 17.346 | 47.521 | 8.741  | 1.00 | 12.21 |
| ATOM | 2594 | N   | SER | 323 | 18.014 | 47.617 | 6.634  | 1.00 | 11.81 |
| ATOM | 2595 | CA  | SER | 323 | 17.069 | 48.683 | 6.345  | 1.00 | 11.28 |
| ATOM | 2596 | CB  | SER | 323 | 17.295 | 49.233 | 4.922  | 1.00 | 14.31 |
| ATOM | 2597 | OG  | SER | 323 | 18.592 | 49.829 | 4.835  | 1.00 | 19.95 |
| ATOM | 2598 | C   | SER | 323 | 15.625 | 48.220 | 6.522  | 1.00 | 11.18 |
| ATOM | 2599 | O   | SER | 323 | 14.776 | 48.982 | 6.976  | 1.00 | 12.09 |
| ATOM | 2600 | N   | LEU | 324 | 15.345 | 46.979 | 6.128  | 1.00 | 11.02 |
| ATOM | 2601 | CA  | LEU | 324 | 13.986 | 46.458 | 6.212  | 1.00 | 9.92  |
| ATOM | 2602 | CB  | LEU | 324 | 13.893 | 45.156 | 5.430  | 1.00 | 9.96  |
| ATOM | 2603 | CG  | LEU | 324 | 12.522 | 44.506 | 5.348  | 1.00 | 9.98  |
| ATOM | 2604 | CD1 | LEU | 324 | 11.448 | 45.393 | 4.776  | 1.00 | 11.33 |
| ATOM | 2605 | CD2 | LEU | 324 | 12.658 | 43.214 | 4.571  | 1.00 | 11.39 |
| ATOM | 2606 | C   | LEU | 324 | 13.576 | 46.326 | 7.679  | 1.00 | 10.28 |
| ATOM | 2607 | O   | LEU | 324 | 12.422 | 46.540 | 8.070  | 1.00 | 10.32 |
| ATOM | 2608 | N   | ILE | 325 | 14.532 | 45.886 | 8.497  | 1.00 | 10.22 |
| ATOM | 2609 | CA  | ILE | 325 | 14.292 | 45.805 | 9.939  | 1.00 | 11.04 |
| ATOM | 2610 | CB  | ILE | 325 | 15.451 | 45.120 | 10.669 | 1.00 | 10.87 |
| ATOM | 2611 | CG2 | ILE | 325 | 15.398 | 45.298 | 12.164 | 1.00 | 13.93 |
| ATOM | 2612 | CG1 | ILE | 325 | 15.454 | 43.605 | 10.363 | 1.00 | 12.46 |
| ATOM | 2613 | CD1 | ILE | 325 | 16.785 | 42.944 | 10.725 | 1.00 | 15.56 |
| ATOM | 2614 | C   | ILE | 325 | 14.040 | 47.192 | 10.522 | 1.00 | 10.74 |
| ATOM | 2615 | O   | ILE | 325 | 13.122 | 47.404 | 11.341 | 1.00 | 11.60 |
| ATOM | 2616 | N   | ASN | 326 | 14.819 | 48.181 | 10.151 | 1.00 | 10.99 |
| ATOM | 2617 | CA  | ASN | 326 | 14.602 | 49.531 | 10.659 | 1.00 | 12.82 |
| ATOM | 2618 | CB  | ASN | 326 | 15.732 | 50.459 | 10.168 | 1.00 | 14.29 |
| ATOM | 2619 | CG  | ASN | 326 | 17.014 | 50.101 | 10.904 | 1.00 | 17.21 |
| ATOM | 2620 | OD1 | ASN | 326 | 16.959 | 49.382 | 11.917 | 1.00 | 23.79 |
| ATOM | 2621 | ND2 | ASN | 326 | 18.130 | 50.520 | 10.318 | 1.00 | 22.06 |
| ATOM | 2622 | C   | ASN | 326 | 13.265 | 50.066 | 10.203 | 1.00 | 12.41 |
| ATOM | 2623 | O   | ASN | 326 | 12.620 | 50.749 | 10.996 | 1.00 | 14.07 |
| ATOM | 2624 | N   | LYS | 327 | 12.840 | 49.790 | 8.973  | 1.00 | 11.71 |

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|      |      |     |     |     |        |        |         |      |       |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2625 | CA  | LYS | 327 | 11.586 | 50.307 | 8.468   | 1.00 | 12.41 |
| ATOM | 2626 | CB  | LYS | 327 | 11.543 | 50.205 | 6.918   | 1.00 | 13.45 |
| ATOM | 2627 | CG  | LYS | 327 | 10.362 | 50.865 | 6.259   | 1.00 | 18.26 |
| ATOM | 2628 | CD  | LYS | 327 | 9.847  | 50.144 | 5.014   | 1.00 | 21.08 |
| ATOM | 2629 | CE  | LYS | 327 | 8.605  | 50.768 | 4.423   | 1.00 | 21.51 |
| ATOM | 2630 | NZ  | LYS | 327 | 7.335  | 50.650 | 5.211   | 1.00 | 17.68 |
| ATOM | 2631 | C   | LYS | 327 | 10.349 | 49.653 | 9.067   | 1.00 | 11.15 |
| ATOM | 2632 | O   | LYS | 327 | 9.389  | 50.327 | 9.506   | 1.00 | 12.52 |
| ATOM | 2633 | N   | ASN | 328 | 10.358 | 48.303 | 8.990   | 1.00 | 10.58 |
| ATOM | 2634 | CA  | ASN | 328 | 9.160  | 47.510 | 9.286   | 1.00 | 11.33 |
| ATOM | 2635 | CB  | ASN | 328 | 8.762  | 46.614 | 8.084   | 1.00 | 14.02 |
| ATOM | 2636 | CG  | ASN | 328 | 8.096  | 47.438 | 7.002   | 1.00 | 14.11 |
| ATOM | 2637 | OD1 | ASN | 328 | 7.997  | 48.681 | 7.112   | 1.00 | 16.02 |
| ATOM | 2638 | ND2 | ASN | 328 | 7.525  | 46.796 | 5.995   | 1.00 | 11.03 |
| ATOM | 2639 | C   | ASN | 328 | 9.224  | 46.671 | 10.551  | 1.00 | 11.26 |
| ATOM | 2640 | O   | ASN | 328 | 8.226  | 45.994 | 10.873  | 1.00 | 13.57 |
| ATOM | 2641 | N   | GLY | 329 | 10.341 | 46.732 | 11.270  | 1.00 | 12.34 |
| ATOM | 2642 | CA  | GLY | 329 | 10.445 | 46.076 | 12.554  | 1.00 | 11.30 |
| ATOM | 2643 | C   | GLY | 329 | 11.146 | 44.739 | 12.523  | 1.00 | 11.94 |
| ATOM | 2644 | O   | GLY | 329 | 11.221 | 44.056 | 11.517  | 1.00 | 11.96 |
| ATOM | 2645 | N   | GLN | 330 | 11.716 | 44.359 | 13.668  | 1.00 | 10.55 |
| ATOM | 2646 | CA  | GLN | 330 | 12.364 | 43.036 | 13.787  | 1.00 | 11.32 |
| ATOM | 2647 | CB  | GLN | 330 | 13.193 | 42.950 | 15.072  | 1.00 | 11.79 |
| ATOM | 2648 | CG  | GLN | 330 | 13.686 | 41.560 | 15.352  | 1.00 | 10.04 |
| ATOM | 2649 | CD  | GLN | 330 | 14.755 | 41.131 | 14.371  | 1.00 | 13.20 |
| ATOM | 2650 | OE1 | GLN | 330 | 15.804 | 41.744 | 14.168  | 1.00 | 11.43 |
| ATOM | 2651 | NE2 | GLN | 330 | 14.469 | 40.024 | 13.733  | 1.00 | 10.94 |
| ATOM | 2652 | C   | GLN | 330 | 11.291 | 41.961 | 13.747  | 1.00 | 12.29 |
| ATOM | 2653 | O   | GLN | 330 | 10.401 | 41.952 | 14.592  | 1.00 | 9.93  |
| ATOM | 2654 | N   | THR | 331 | 11.377 | 41.063 | 12.784  | 1.00 | 10.56 |
| ATOM | 2655 | CA  | THR | 331 | 10.438 | 39.956 | 12.692  | 1.00 | 13.12 |
| ATOM | 2656 | CB  | THR | 331 | 10.367 | 39.375 | 11.277  | 1.00 | 14.79 |
| ATOM | 2657 | OG1 | THR | 331 | 11.627 | 38.829 | 10.872  | 1.00 | 18.32 |
| ATOM | 2658 | CG2 | THR | 331 | 9.945  | 40.455 | 10.274  | 1.00 | 9.68  |
| ATOM | 2659 | C   | THR | 331 | 10.801 | 38.843 | 13.669  | 1.00 | 10.45 |
| ATOM | 2660 | O   | THR | 331 | 9.996  | 37.874 | 13.694  | 1.00 | 9.25  |
| ATOM | 2661 | OT  | THR | 331 | 11.803 | 38.971 | 14.419  | 1.00 | 6.49  |
| ATOM | 2662 | OW  | WAT | 334 | 9.679  | 28.766 | -0.715  | 1.00 | 7.24  |
| ATOM | 2663 | OW  | WAT | 335 | 19.171 | 27.783 | 10.936  | 1.00 | 8.08  |
| ATOM | 2664 | OW  | WAT | 335 | 9.260  | 43.735 | -4.195  | 1.00 | 6.26  |
| ATOM | 2665 | OW  | WAT | 336 | 22.532 | 31.208 | 2.029   | 1.00 | 7.97  |
| ATOM | 2666 | OW  | WAT | 337 | 28.595 | 34.041 | 1.151   | 1.00 | 8.47  |
| ATOM | 2667 | OW  | WAT | 338 | 24.607 | 26.075 | 6.861   | 1.00 | 8.55  |
| ATOM | 2668 | OW  | WAT | 339 | -2.784 | 36.461 | -0.561  | 1.00 | 7.69  |
| ATOM | 2669 | OW  | WAT | 340 | 22.156 | 23.031 | 7.059   | 1.00 | 8.58  |
| ATOM | 2670 | OW  | WAT | 341 | 14.777 | 39.110 | 1.828   | 1.00 | 9.25  |
| ATOM | 2671 | OW  | WAT | 342 | 12.607 | 41.059 | 1.589   | 1.00 | 9.09  |
| ATOM | 2672 | OW  | WAT | 343 | -1.547 | 35.753 | 12.742  | 1.00 | 8.72  |
| ATOM | 2673 | OW  | WAT | 344 | 15.859 | 16.926 | 12.366  | 1.00 | 8.11  |
| ATOM | 2674 | OW  | WAT | 345 | 17.270 | 37.486 | 2.078   | 1.00 | 10.08 |
| ATOM | 2675 | OW  | WAT | 346 | 3.657  | 33.965 | -24.602 | 1.00 | 9.87  |
| ATOM | 2676 | OW  | WAT | 347 | 25.532 | 21.232 | -3.227  | 1.00 | 9.24  |
| ATOM | 2677 | OW  | WAT | 348 | -2.697 | 35.006 | 10.127  | 1.00 | 9.83  |
| ATOM | 2678 | OW  | WAT | 349 | -1.983 | 38.149 | 8.911   | 1.00 | 10.06 |
| ATOM | 2679 | OW  | WAT | 350 | 2.708  | 25.709 | 10.377  | 1.00 | 10.39 |
| ATOM | 2680 | OW  | WAT | 351 | 1.466  | 29.802 | -2.581  | 1.00 | 10.21 |
| ATOM | 2681 | OW  | WAT | 352 | 1.694  | 36.486 | 5.140   | 1.00 | 11.32 |
| ATOM | 2682 | OW  | WAT | 353 | 14.787 | 40.054 | -27.891 | 1.00 | 11.49 |
| ATOM | 2683 | OW  | WAT | 354 | 7.944  | 41.566 | -10.080 | 1.00 | 11.45 |
| ATOM | 2684 | OW  | WAT | 355 | 10.898 | 19.364 | -0.933  | 1.00 | 10.27 |
| ATOM | 2685 | OW  | WAT | 356 | 11.246 | 44.075 | 8.852   | 1.00 | 12.14 |
| ATOM | 2686 | OW  | WAT | 357 | 19.835 | 30.921 | -23.876 | 1.00 | 10.92 |
| ATOM | 2687 | OW  | WAT | 358 | 27.717 | 21.786 | -4.790  | 1.00 | 11.81 |
| ATOM | 2688 | OW  | WAT | 359 | 25.375 | 32.089 | -5.869  | 1.00 | 10.99 |
| ATOM | 2689 | OW  | WAT | 360 | 7.719  | 32.045 | 19.976  | 1.00 | 10.19 |
| ATOM | 2690 | OW  | WAT | 361 | 12.903 | 41.900 | 8.252   | 1.00 | 10.84 |
| ATOM | 2691 | OW  | WAT | 362 | 15.465 | 41.811 | 7.221   | 1.00 | 12.37 |
| ATOM | 2692 | OW  | WAT | 363 | 12.347 | 17.857 | 1.029   | 1.00 | 10.86 |
| ATOM | 2693 | OW  | WAT | 364 | 16.302 | 36.649 | -24.739 | 1.00 | 12.28 |
| ATOM | 2694 | OW  | WAT | 365 | 10.865 | 30.651 | 24.027  | 1.00 | 10.14 |
| ATOM | 2695 | OW  | WAT | 366 | 19.416 | 33.418 | -15.771 | 1.00 | 11.04 |
| ATOM | 2696 | OW  | WAT | 367 | 0.655  | 27.761 | 10.957  | 1.00 | 11.14 |
| ATOM | 2697 | OW  | WAT | 368 | 6.259  | 36.234 | -3.794  | 1.00 |       |

|      |      |    |     |     |        |        |         |      |       |
|------|------|----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2698 | OW | WAT | 369 | 16.675 | 14.973 | 9.695   | 1.00 | 11.88 |
| ATOM | 2699 | OW | WAT | 370 | 7.905  | 39.248 | -11.909 | 1.00 | 10.25 |
| ATOM | 2700 | OW | WAT | 371 | 18.361 | 15.936 | 2.863   | 1.00 | 11.46 |
| ATOM | 2701 | OW | WAT | 372 | 21.892 | 19.503 | 1.831   | 1.00 | 13.37 |
| ATOM | 2702 | OW | WAT | 373 | 7.417  | 33.809 | 23.230  | 1.00 | 11.13 |
| ATOM | 2703 | OW | WAT | 374 | 9.301  | 18.255 | -4.039  | 1.00 | 13.47 |
| ATOM | 2704 | OW | WAT | 375 | 5.788  | 38.293 | -2.097  | 1.00 | 12.75 |
| ATOM | 2705 | OW | WAT | 376 | 21.318 | 28.084 | 18.230  | 1.00 | 13.18 |
| ATOM | 2706 | OW | WAT | 377 | 5.087  | 41.215 | -22.821 | 1.00 | 13.37 |
| ATOM | 2707 | OW | WAT | 378 | 24.969 | 23.273 | 6.991   | 1.00 | 13.42 |
| ATOM | 2708 | OW | WAT | 379 | 11.227 | 49.320 | -8.022  | 1.00 | 13.43 |
| ATOM | 2709 | OW | WAT | 380 | -7.291 | 29.246 | 11.626  | 1.00 | 13.60 |
| ATOM | 2710 | OW | WAT | 381 | 5.640  | 46.235 | 9.550   | 1.00 | 13.85 |
| ATOM | 2711 | OW | WAT | 382 | 8.978  | 35.948 | 12.107  | 1.00 | 11.77 |
| ATOM | 2712 | OW | WAT | 383 | 6.906  | 29.370 | 22.628  | 1.00 | 15.24 |
| ATOM | 2713 | OW | WAT | 384 | 9.627  | 19.425 | 20.724  | 1.00 | 14.52 |
| ATOM | 2714 | OW | WAT | 385 | 16.459 | 39.497 | 8.314   | 1.00 | 14.01 |
| ATOM | 2715 | OW | WAT | 386 | 24.545 | 45.847 | -10.066 | 1.00 | 13.62 |
| ATOM | 2716 | OW | WAT | 387 | -0.150 | 40.151 | 13.142  | 1.00 | 15.04 |
| ATOM | 2717 | OW | WAT | 388 | 17.528 | 29.411 | -23.847 | 1.00 | 12.67 |
| ATOM | 2718 | OW | WAT | 389 | 11.478 | 50.549 | -25.585 | 1.00 | 14.89 |
| ATOM | 2719 | OW | WAT | 390 | 13.559 | 40.717 | 10.705  | 1.00 | 15.14 |
| ATOM | 2720 | OW | WAT | 391 | 8.290  | 18.854 | -0.320  | 1.00 | 13.36 |
| ATOM | 2721 | OW | WAT | 392 | 18.743 | 43.137 | -23.378 | 1.00 | 14.45 |
| ATOM | 2722 | OW | WAT | 393 | -0.660 | 20.811 | -4.126  | 1.00 | 13.51 |
| ATOM | 2723 | OW | WAT | 394 | 11.073 | 48.625 | 1.433   | 1.00 | 16.03 |
| ATOM | 2724 | OW | WAT | 395 | 21.541 | 28.028 | -11.200 | 1.00 | 13.36 |
| ATOM | 2725 | OW | WAT | 396 | -9.012 | 33.285 | 2.180   | 1.00 | 14.72 |
| ATOM | 2726 | OW | WAT | 397 | -5.015 | 37.842 | -7.595  | 1.00 | 13.04 |
| ATOM | 2727 | OW | WAT | 398 | 7.685  | 39.106 | -0.476  | 1.00 | 15.18 |
| ATOM | 2728 | OW | WAT | 399 | -2.609 | 52.730 | 2.926   | 1.00 | 15.90 |
| ATOM | 2729 | OW | WAT | 400 | 31.148 | 33.765 | -2.024  | 1.00 | 14.37 |
| ATOM | 2730 | OW | WAT | 401 | 28.412 | 25.681 | -6.948  | 1.00 | 16.42 |
| ATOM | 2731 | OW | WAT | 402 | -7.837 | 33.960 | -2.251  | 1.00 | 16.15 |
| ATOM | 2732 | OW | WAT | 403 | 27.733 | 30.817 | 11.858  | 1.00 | 15.84 |
| ATOM | 2733 | OW | WAT | 404 | 20.345 | 47.455 | -0.111  | 1.00 | 15.47 |
| ATOM | 2734 | OW | WAT | 405 | 7.740  | 46.885 | -13.836 | 1.00 | 13.61 |
| ATOM | 2735 | OW | WAT | 406 | -6.948 | 43.028 | 7.219   | 1.00 | 15.03 |
| ATOM | 2736 | OW | WAT | 407 | -1.255 | 31.160 | -1.492  | 1.00 | 16.57 |
| ATOM | 2737 | OW | WAT | 408 | -7.351 | 47.298 | 1.758   | 1.00 | 13.70 |
| ATOM | 2738 | OW | WAT | 409 | 0.600  | 50.511 | 3.412   | 1.00 | 13.82 |
| ATOM | 2739 | OW | WAT | 410 | 19.491 | 38.870 | 14.832  | 1.00 | 12.61 |
| ATOM | 2740 | OW | WAT | 411 | 19.032 | 29.394 | 25.238  | 1.00 | 16.16 |
| ATOM | 2741 | OW | WAT | 412 | 1.566  | 19.249 | -3.495  | 1.00 | 17.83 |
| ATOM | 2742 | OW | WAT | 413 | 1.396  | 29.458 | -19.005 | 1.00 | 16.00 |
| ATOM | 2743 | OW | WAT | 414 | 12.993 | 13.760 | 6.156   | 1.00 | 14.57 |
| ATOM | 2744 | OW | WAT | 415 | -3.489 | 25.740 | 2.588   | 1.00 | 15.12 |
| ATOM | 2745 | OW | WAT | 416 | 20.400 | 16.258 | 4.749   | 1.00 | 16.18 |
| ATOM | 2746 | OW | WAT | 417 | 8.420  | 43.590 | -11.863 | 1.00 | 15.01 |
| ATOM | 2747 | OW | WAT | 418 | 23.155 | 21.243 | -4.704  | 1.00 | 18.08 |
| ATOM | 2748 | OW | WAT | 419 | 13.407 | 49.512 | -6.246  | 1.00 | 15.55 |
| ATOM | 2749 | OW | WAT | 420 | 2.293  | 43.872 | -19.188 | 1.00 | 16.03 |
| ATOM | 2750 | OW | WAT | 421 | 16.464 | 23.984 | -12.729 | 1.00 | 16.50 |
| ATOM | 2751 | OW | WAT | 422 | 18.051 | 18.401 | 13.304  | 1.00 | 15.75 |
| ATOM | 2752 | OW | WAT | 423 | 2.749  | 32.610 | 17.294  | 1.00 | 16.03 |
| ATOM | 2753 | OW | WAT | 424 | 3.167  | 43.048 | -21.870 | 1.00 | 16.60 |
| ATOM | 2754 | OW | WAT | 425 | 1.729  | 36.092 | 20.156  | 1.00 | 17.06 |
| ATOM | 2755 | OW | WAT | 426 | 24.912 | 30.437 | 18.039  | 1.00 | 18.10 |
| ATOM | 2756 | OW | WAT | 427 | 1.661  | 37.179 | -17.778 | 1.00 | 16.68 |
| ATOM | 2757 | OW | WAT | 428 | 8.377  | 48.751 | -17.456 | 1.00 | 17.96 |
| ATOM | 2758 | OW | WAT | 429 | 4.193  | 48.686 | -6.577  | 1.00 | 16.18 |
| ATOM | 2759 | OW | WAT | 430 | 32.183 | 20.100 | 4.650   | 1.00 | 17.47 |
| ATOM | 2760 | OW | WAT | 431 | 10.701 | 20.889 | -9.309  | 1.00 | 17.06 |
| ATOM | 2761 | OW | WAT | 432 | 1.230  | 36.624 | -21.785 | 1.00 | 16.21 |
| ATOM | 2762 | OW | WAT | 433 | 23.224 | 53.219 | -9.124  | 1.00 | 16.77 |
| ATOM | 2763 | OW | WAT | 434 | 7.454  | 14.204 | -2.641  | 1.00 | 19.16 |
| ATOM | 2764 | OW | WAT | 435 | -3.493 | 18.204 | -1.008  | 1.00 | 16.26 |
| ATOM | 2765 | OW | WAT | 436 | 28.871 | 35.527 | -9.186  | 1.00 | 16.44 |
| ATOM | 2766 | OW | WAT | 437 | 28.827 | 47.359 | -4.440  | 1.00 | 20.15 |
| ATOM | 2767 | OW | WAT | 438 | 16.179 | 24.748 | -15.541 | 1.00 | 18.41 |
| ATOM | 2768 | OW | WAT | 439 | 24.130 | 23.189 | 10.125  | 1.00 | 15.71 |
| ATOM | 2769 | OW | WAT | 440 | 9.413  | 18.353 | 13.315  | 1.00 | 22.18 |
| ATOM | 2770 | OW | WAT | 441 | 8.848  | 18.233 | 10.527  | 1.00 | 19.65 |

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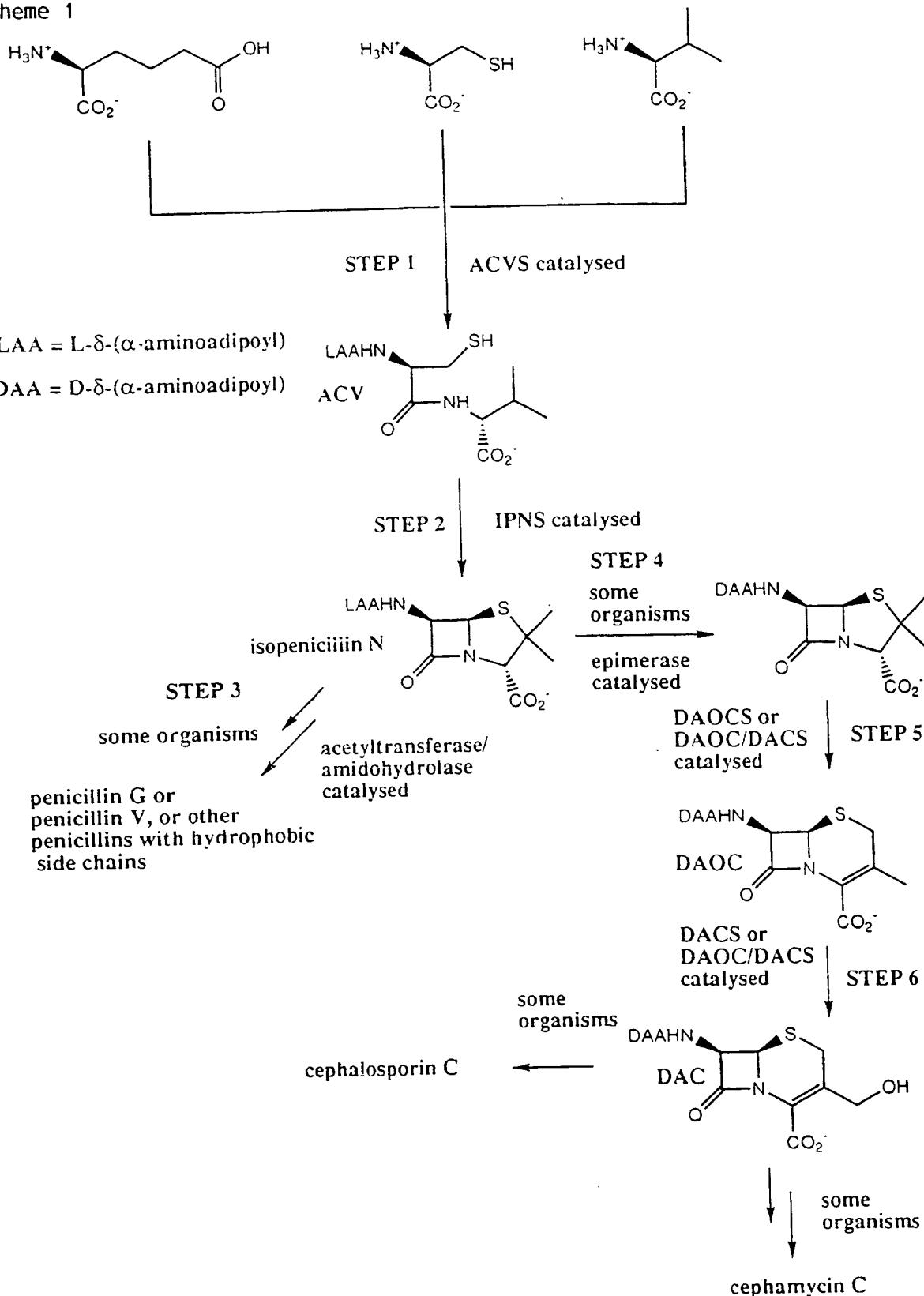
|      |      |    |     |     |         |        |         |      |       |
|------|------|----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 2771 | OW | WAT | 442 | 26.464  | 32.534 | 18.217  | 1.00 | 16.18 |
| ATOM | 2772 | OW | WAT | 443 | -7.877  | 38.342 | 4.061   | 1.00 | 17.91 |
| ATOM | 2773 | OW | WAT | 444 | 12.963  | 34.080 | 10.130  | 1.00 | 14.21 |
| ATOM | 2774 | OW | WAT | 445 | 5.117   | 27.600 | 16.871  | 1.00 | 17.53 |
| ATOM | 2775 | OW | WAT | 446 | -9.839  | 37.847 | 2.096   | 1.00 | 20.90 |
| ATOM | 2776 | OW | WAT | 447 | -1.745  | 32.409 | 3.793   | 1.00 | 20.56 |
| ATOM | 2777 | OW | WAT | 448 | 8.416   | 36.915 | 9.538   | 1.00 | 19.37 |
| ATOM | 2778 | OW | WAT | 449 | 13.442  | 46.906 | 0.805   | 1.00 | 15.63 |
| ATOM | 2779 | OW | WAT | 450 | 4.457   | 30.452 | 20.352  | 1.00 | 16.16 |
| ATOM | 2780 | OW | WAT | 451 | 8.792   | 16.265 | -0.627  | 1.00 | 17.14 |
| ATOM | 2781 | OW | WAT | 452 | -0.356  | 37.156 | 21.516  | 1.00 | 17.26 |
| ATOM | 2782 | OW | WAT | 453 | 11.477  | 23.152 | -22.757 | 1.00 | 21.00 |
| ATOM | 2783 | OW | WAT | 454 | 21.490  | 29.901 | 24.676  | 1.00 | 18.12 |
| ATOM | 2784 | OW | WAT | 455 | -9.438  | 38.109 | 10.367  | 1.00 | 20.23 |
| ATOM | 2785 | OW | WAT | 456 | 0.801   | 21.803 | -6.497  | 1.00 | 16.76 |
| ATOM | 2786 | OW | WAT | 457 | 19.962  | 49.749 | -14.695 | 1.00 | 19.53 |
| ATOM | 2787 | OW | WAT | 458 | 15.665  | 20.950 | 19.711  | 1.00 | 20.63 |
| ATOM | 2788 | OW | WAT | 459 | 22.253  | 42.588 | 7.507   | 1.00 | 18.83 |
| ATOM | 2789 | OW | WAT | 460 | 1.091   | 15.140 | -0.991  | 1.00 | 17.62 |
| ATOM | 2790 | OW | WAT | 461 | 15.096  | 47.428 | -1.171  | 1.00 | 18.28 |
| ATOM | 2791 | OW | WAT | 462 | 9.229   | 16.847 | 19.798  | 1.00 | 19.90 |
| ATOM | 2792 | OW | WAT | 463 | 23.458  | 31.087 | 12.465  | 1.00 | 20.21 |
| ATOM | 2793 | OW | WAT | 464 | 19.997  | 42.399 | 9.231   | 1.00 | 20.50 |
| ATOM | 2794 | OW | WAT | 465 | -1.338  | 22.340 | -1.994  | 1.00 | 18.86 |
| ATOM | 2795 | OW | WAT | 466 | 3.252   | 20.298 | -7.395  | 1.00 | 20.44 |
| ATOM | 2796 | OW | WAT | 467 | 13.042  | 53.167 | -27.095 | 1.00 | 19.91 |
| ATOM | 2797 | OW | WAT | 468 | -10.643 | 37.955 | 15.133  | 1.00 | 20.65 |
| ATOM | 2798 | OW | WAT | 469 | 13.185  | 21.680 | -8.488  | 1.00 | 20.52 |
| ATOM | 2799 | OW | WAT | 470 | 10.293  | 15.611 | 9.484   | 1.00 | 17.30 |
| ATOM | 2800 | OW | WAT | 471 | 18.301  | 39.511 | -27.728 | 1.00 | 15.98 |
| ATOM | 2801 | OW | WAT | 472 | 30.497  | 24.989 | -0.891  | 1.00 | 18.92 |
| ATOM | 2802 | OW | WAT | 473 | 34.106  | 27.545 | 11.353  | 1.00 | 20.62 |
| ATOM | 2803 | OW | WAT | 474 | -1.263  | 34.235 | -1.003  | 1.00 | 21.04 |
| ATOM | 2804 | OW | WAT | 475 | 30.740  | 34.281 | 8.033   | 1.00 | 22.42 |
| ATOM | 2805 | OW | WAT | 476 | 17.888  | 47.600 | -24.851 | 1.00 | 19.76 |
| ATOM | 2806 | OW | WAT | 477 | 19.023  | 45.815 | -22.920 | 1.00 | 19.37 |
| ATOM | 2807 | OW | WAT | 478 | 5.376   | 27.996 | -23.488 | 1.00 | 23.73 |
| ATOM | 2808 | OW | WAT | 479 | 18.268  | 40.811 | 13.239  | 1.00 | 19.22 |
| ATOM | 2809 | OW | WAT | 480 | -4.271  | 44.290 | -11.498 | 1.00 | 18.91 |
| ATOM | 2810 | OW | WAT | 481 | -10.443 | 35.240 | 1.254   | 1.00 | 19.18 |
| ATOM | 2811 | OW | WAT | 482 | 2.681   | 33.500 | 20.144  | 1.00 | 20.32 |
| ATOM | 2812 | OW | WAT | 483 | 19.770  | 15.947 | 12.144  | 1.00 | 21.46 |
| ATOM | 2813 | OW | WAT | 484 | 4.713   | 13.467 | 7.499   | 1.00 | 23.32 |
| ATOM | 2814 | OW | WAT | 485 | -8.355  | 31.805 | -0.398  | 1.00 | 18.04 |
| ATOM | 2815 | OW | WAT | 486 | 15.331  | 47.230 | 2.640   | 1.00 | 23.97 |
| ATOM | 2816 | OW | WAT | 487 | 25.206  | 36.975 | 8.919   | 1.00 | 18.16 |
| ATOM | 2817 | OW | WAT | 488 | 2.787   | 39.754 | 14.409  | 1.00 | 21.20 |
| ATOM | 2818 | OW | WAT | 489 | 2.364   | 46.924 | -9.024  | 1.00 | 19.59 |
| ATOM | 2819 | OW | WAT | 490 | 18.912  | 42.320 | -26.268 | 1.00 | 22.28 |
| ATOM | 2820 | OW | WAT | 491 | 9.332   | 14.150 | -7.989  | 1.00 | 20.14 |
| ATOM | 2821 | OW | WAT | 492 | 3.716   | 51.522 | -5.917  | 1.00 | 22.71 |
| ATOM | 2822 | OW | WAT | 493 | 30.485  | 19.369 | 6.691   | 1.00 | 21.63 |
| ATOM | 2823 | OW | WAT | 494 | -8.748  | 45.801 | 7.529   | 1.00 | 21.66 |
| ATOM | 2824 | OW | WAT | 495 | 11.868  | 16.205 | -2.683  | 1.00 | 19.24 |
| ATOM | 2825 | OW | WAT | 496 | 13.346  | 35.997 | 8.497   | 1.00 | 21.95 |
| ATOM | 2826 | OW | WAT | 497 | 0.972   | 40.899 | -13.028 | 1.00 | 28.32 |
| ATOM | 2827 | OW | WAT | 498 | 4.183   | 53.535 | -1.459  | 1.00 | 20.11 |
| ATOM | 2828 | OW | WAT | 499 | 30.346  | 39.016 | -10.546 | 1.00 | 25.21 |
| ATOM | 2829 | OW | WAT | 500 | 16.129  | 24.513 | -19.240 | 1.00 | 28.12 |
| ATOM | 2830 | OW | WAT | 501 | 10.923  | 41.632 | 17.779  | 1.00 | 22.89 |
| ATOM | 2831 | OW | WAT | 502 | 18.809  | 24.865 | -19.164 | 1.00 | 19.20 |
| ATOM | 2832 | OW | WAT | 503 | 16.648  | 14.113 | 0.751   | 1.00 | 20.79 |
| ATOM | 2833 | OW | WAT | 504 | 19.213  | 39.701 | 8.979   | 1.00 | 20.81 |
| ATOM | 2834 | OW | WAT | 505 | 24.711  | 56.540 | -10.148 | 1.00 | 22.77 |
| ATOM | 2835 | OW | WAT | 506 | 22.101  | 29.548 | -23.677 | 1.00 | 24.26 |
| ATOM | 2836 | OW | WAT | 507 | 21.631  | 41.072 | 20.961  | 1.00 | 25.98 |
| ATOM | 2837 | OW | WAT | 508 | -3.925  | 32.996 | -15.355 | 1.00 | 23.91 |
| ATOM | 2838 | OW | WAT | 509 | -3.683  | 27.982 | 6.567   | 1.00 | 24.78 |
| ATOM | 2839 | OW | WAT | 510 | 22.548  | 22.934 | 15.189  | 1.00 | 21.05 |
| ATOM | 2840 | OW | WAT | 511 | 3.233   | 21.643 | -9.764  | 1.00 | 24.54 |
| ATOM | 2841 | OW | WAT | 512 | 33.443  | 23.225 | 2.328   | 1.00 | 25.43 |
| ATOM | 2842 | OW | WAT | 513 | 24.602  | 43.728 | -18.078 | 1.00 | 22.61 |
| ATOM | 2843 | OW | WAT | 514 | 16.686  | 43.816 | 15.797  | 1.00 |       |

|      |      |    |     |     |         |        |         |      |       |
|------|------|----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 2844 | OW | WAT | 515 | 10.964  | 18.976 | -6.714  | 1.00 | 26.05 |
| ATOM | 2845 | OW | WAT | 516 | 0.840   | 16.582 | -3.289  | 1.00 | 22.32 |
| ATOM | 2846 | OW | WAT | 517 | -3.923  | 22.464 | -1.744  | 1.00 | 29.01 |
| ATOM | 2847 | OW | WAT | 518 | -0.997  | 25.906 | 9.408   | 1.00 | 27.67 |
| ATOM | 2848 | OW | WAT | 519 | 3.066   | 45.067 | -23.581 | 1.00 | 21.23 |
| ATOM | 2849 | OW | WAT | 520 | 20.631  | 16.301 | 16.915  | 1.00 | 29.84 |
| ATOM | 2850 | OW | WAT | 521 | 3.683   | 28.042 | -20.317 | 1.00 | 29.99 |
| ATOM | 2851 | OW | WAT | 522 | -7.926  | 27.757 | 3.844   | 1.00 | 23.89 |
| ATOM | 2852 | OW | WAT | 523 | 1.150   | 23.857 | -9.846  | 1.00 | 21.74 |
| ATOM | 2853 | OW | WAT | 524 | 13.889  | 16.199 | -5.074  | 1.00 | 22.55 |
| ATOM | 2854 | OW | WAT | 525 | -1.704  | 53.692 | -2.952  | 1.00 | 32.09 |
| ATOM | 2855 | OW | WAT | 526 | 30.576  | 35.496 | -4.718  | 1.00 | 26.56 |
| ATOM | 2856 | OW | WAT | 527 | 7.959   | 27.774 | -32.333 | 1.00 | 22.85 |
| ATOM | 2857 | OW | WAT | 528 | 0.310   | 39.649 | -17.650 | 1.00 | 26.17 |
| ATOM | 2858 | OW | WAT | 529 | -0.573  | 40.681 | -15.285 | 1.00 | 24.02 |
| ATOM | 2859 | OW | WAT | 530 | -5.413  | 37.314 | -11.579 | 1.00 | 26.13 |
| ATOM | 2860 | OW | WAT | 531 | 20.453  | 25.296 | -22.221 | 1.00 | 26.01 |
| ATOM | 2861 | OW | WAT | 532 | 2.287   | 15.472 | -5.046  | 1.00 | 27.90 |
| ATOM | 2862 | OW | WAT | 533 | 30.000  | 42.526 | -1.756  | 1.00 | 25.99 |
| ATOM | 2863 | OW | WAT | 534 | 13.014  | 48.338 | 13.867  | 1.00 | 29.93 |
| ATOM | 2864 | OW | WAT | 535 | 19.089  | 59.470 | -16.490 | 1.00 | 25.60 |
| ATOM | 2865 | OW | WAT | 536 | 23.246  | 37.608 | -22.518 | 1.00 | 30.37 |
| ATOM | 2866 | OW | WAT | 537 | 18.012  | 23.775 | -22.832 | 1.00 | 35.14 |
| ATOM | 2867 | OW | WAT | 538 | 32.942  | 31.103 | -1.587  | 1.00 | 27.55 |
| ATOM | 2868 | OW | WAT | 539 | 24.244  | 39.395 | 8.376   | 1.00 | 26.84 |
| ATOM | 2869 | OW | WAT | 540 | 16.151  | 39.516 | 11.126  | 1.00 | 27.39 |
| ATOM | 2870 | OW | WAT | 541 | -9.496  | 38.640 | 6.232   | 1.00 | 23.00 |
| ATOM | 2871 | OW | WAT | 542 | 11.570  | 53.681 | -24.197 | 1.00 | 25.04 |
| ATOM | 2872 | OW | WAT | 543 | 5.652   | 39.623 | 9.901   | 1.00 | 24.86 |
| ATOM | 2873 | OW | WAT | 544 | 15.243  | 51.336 | -7.590  | 1.00 | 31.58 |
| ATOM | 2874 | OW | WAT | 545 | 21.732  | 45.731 | -22.796 | 1.00 | 25.40 |
| ATOM | 2875 | OW | WAT | 546 | 26.109  | 29.562 | 15.747  | 1.00 | 26.48 |
| ATOM | 2876 | OW | WAT | 547 | 5.300   | 48.774 | 10.712  | 1.00 | 22.97 |
| ATOM | 2877 | OW | WAT | 548 | 16.333  | 19.082 | -6.041  | 1.00 | 31.87 |
| ATOM | 2878 | OW | WAT | 549 | 34.477  | 39.693 | -0.433  | 1.00 | 24.27 |
| ATOM | 2879 | OW | WAT | 550 | 32.307  | 28.802 | -2.454  | 1.00 | 28.07 |
| ATOM | 2880 | OW | WAT | 551 | 16.750  | 23.348 | 20.119  | 1.00 | 30.93 |
| ATOM | 2881 | OW | WAT | 552 | 19.254  | 45.692 | 25.110  | 1.00 | 31.35 |
| ATOM | 2882 | OW | WAT | 553 | 7.615   | 43.287 | 12.031  | 1.00 | 24.54 |
| ATOM | 2883 | OW | WAT | 554 | 21.139  | 41.273 | 15.275  | 1.00 | 28.18 |
| ATOM | 2884 | OW | WAT | 555 | -9.531  | 43.159 | 1.000   | 1.00 | 25.96 |
| ATOM | 2885 | OW | WAT | 556 | -4.562  | 35.560 | 22.961  | 1.00 | 29.93 |
| ATOM | 2886 | OW | WAT | 557 | 19.748  | 24.192 | -10.428 | 1.00 | 27.47 |
| ATOM | 2887 | OW | WAT | 558 | 10.358  | 13.845 | 7.421   | 1.00 | 27.41 |
| ATOM | 2888 | OW | WAT | 559 | 33.144  | 26.300 | -1.473  | 1.00 | 23.51 |
| ATOM | 2889 | OW | WAT | 560 | 0.711   | 42.085 | -22.328 | 1.00 | 27.47 |
| ATOM | 2890 | OW | WAT | 561 | 19.258  | 55.289 | -14.564 | 1.00 | 25.35 |
| ATOM | 2891 | OW | WAT | 562 | 13.683  | 49.398 | -2.033  | 1.00 | 27.95 |
| ATOM | 2892 | OW | WAT | 563 | 21.974  | 39.944 | 7.537   | 1.00 | 24.21 |
| ATOM | 2893 | OW | WAT | 564 | 14.094  | 24.261 | -29.685 | 1.00 | 30.81 |
| ATOM | 2894 | OW | WAT | 565 | 8.391   | 16.742 | 16.583  | 1.00 | 33.63 |
| ATOM | 2895 | OW | WAT | 566 | 34.902  | 40.206 | 3.922   | 1.00 | 34.09 |
| ATOM | 2896 | OW | WAT | 567 | 7.246   | 39.309 | 7.727   | 1.00 | 25.05 |
| ATOM | 2897 | OW | WAT | 568 | 1.772   | 52.043 | -7.936  | 1.00 | 33.11 |
| ATOM | 2898 | OW | WAT | 569 | -10.176 | 35.406 | -1.420  | 1.00 | 28.71 |
| ATOM | 2899 | OW | WAT | 570 | 19.034  | 21.727 | -6.972  | 1.00 | 31.14 |
| ATOM | 2900 | OW | WAT | 571 | 25.186  | 25.032 | 13.807  | 1.00 | 29.45 |
| ATOM | 2901 | OW | WAT | 572 | -0.477  | 22.506 | 0.681   | 1.00 | 29.75 |
| ATOM | 2902 | OW | WAT | 573 | 7.554   | 13.615 | 9.613   | 1.00 | 25.51 |
| ATOM | 2903 | OW | WAT | 574 | 0.741   | 15.993 | -6.797  | 1.00 | 28.22 |
| ATOM | 2904 | OW | WAT | 575 | 4.524   | 26.932 | 19.683  | 1.00 | 30.25 |
| ATOM | 2905 | OW | WAT | 576 | 24.217  | 31.560 | 29.964  | 1.00 | 30.98 |
| ATOM | 2906 | OW | WAT | 577 | -9.886  | 38.987 | -0.391  | 1.00 | 30.58 |
| ATOM | 2907 | OW | WAT | 578 | 18.264  | 48.710 | -5.256  | 1.00 | 26.25 |
| ATOM | 2908 | OW | WAT | 579 | 7.094   | 48.558 | -19.857 | 1.00 | 30.55 |
| ATOM | 2909 | OW | WAT | 580 | -11.403 | 38.772 | 12.578  | 1.00 | 23.49 |
| ATOM | 2910 | OW | WAT | 581 | 0.236   | 53.067 | 3.666   | 1.00 | 32.85 |
| ATOM | 2911 | OW | WAT | 582 | 34.494  | 30.211 | 11.953  | 1.00 | 30.38 |
| ATOM | 2912 | OW | WAT | 583 | -8.883  | 40.085 | 8.563   | 1.00 | 20.61 |
| ATOM | 2913 | OW | WAT | 584 | 19.648  | 16.274 | -1.256  | 1.00 | 32.05 |
| ATOM | 2914 | OW | WAT | 585 | 0.789   | 53.240 | 6.163   | 1.00 | 28.48 |
| ATOM | 2915 | OW | WAT | 586 | 6.772   | 16.061 | 19.133  | 1.00 | 28.67 |
| ATOM | 2916 | OW | WAT | 587 | 17.572  | 48.350 | -0.455  | 1.00 | 31.70 |

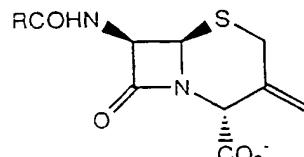
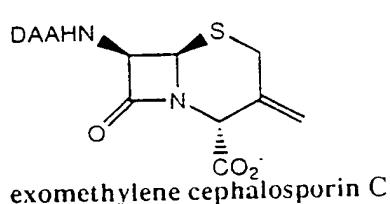
| ATOM | 2917 | OW | WAT | 588 | 19.914  | 42.743 | 12.082  | 1.00 | 29.47 |
|------|------|----|-----|-----|---------|--------|---------|------|-------|
| ATOM | 2918 | OW | WAT | 589 | 28.293  | 43.369 | 3.095   | 1.00 | 41.10 |
| ATOM | 2919 | OW | WAT | 590 | 4.140   | 16.905 | -6.015  | 1.00 | 33.04 |
| ATOM | 2920 | OW | WAT | 591 | -7.536  | 49.473 | 0.700   | 1.00 | 26.21 |
| ATOM | 2921 | OW | WAT | 592 | 16.545  | 11.527 | 7.703   | 1.00 | 35.77 |
| ATOM | 2922 | OW | WAT | 593 | 21.751  | 26.587 | -18.455 | 1.00 | 36.98 |
| ATOM | 2923 | OW | WAT | 594 | 28.027  | 36.486 | 9.408   | 1.00 | 30.24 |
| ATOM | 2924 | OW | WAT | 595 | -3.668  | 27.781 | 16.465  | 1.00 | 32.59 |
| ATOM | 2925 | OW | WAT | 596 | 6.641   | 50.716 | 9.132   | 1.00 | 30.57 |
| ATOM | 2926 | OW | WAT | 597 | 14.904  | 54.419 | -12.497 | 1.00 | 35.34 |
| ATOM | 2927 | OW | WAT | 598 | 13.687  | 41.518 | 18.737  | 1.00 | 28.20 |
| ATOM | 2928 | OW | WAT | 599 | 15.809  | 10.449 | 13.628  | 1.00 | 27.51 |
| ATOM | 2929 | OW | WAT | 600 | 0.266   | 35.585 | -19.094 | 1.00 | 32.22 |
| ATOM | 2930 | OW | WAT | 601 | 1.157   | 32.250 | -2.186  | 1.00 | 31.93 |
| ATOM | 2931 | OW | WAT | 602 | 20.830  | 54.594 | -22.978 | 1.00 | 38.78 |
| ATOM | 2932 | OW | WAT | 603 | -6.482  | 24.335 | 0.209   | 1.00 | 27.40 |
| ATOM | 2933 | OW | WAT | 604 | -0.221  | 24.757 | -19.652 | 1.00 | 34.87 |
| ATOM | 2934 | OW | WAT | 605 | 4.475   | 41.359 | 13.507  | 1.00 | 38.95 |
| ATOM | 2935 | OW | WAT | 606 | 18.365  | 17.118 | -5.002  | 1.00 | 35.63 |
| ATOM | 2936 | OW | WAT | 607 | 10.129  | 37.103 | 7.607   | 1.00 | 37.59 |
| ATOM | 2937 | OW | WAT | 608 | 32.483  | 26.313 | -6.257  | 1.00 | 34.83 |
| ATOM | 2938 | OW | WAT | 609 | 1.173   | 18.896 | 13.815  | 1.00 | 38.79 |
| ATOM | 2939 | OW | WAT | 610 | 21.714  | 21.650 | -7.187  | 1.00 | 30.79 |
| ATOM | 2940 | OW | WAT | 611 | 16.630  | 13.196 | 3.673   | 1.00 | 38.22 |
| ATOM | 2941 | OW | WAT | 612 | 3.332   | 18.798 | 15.551  | 1.00 | 30.36 |
| ATOM | 2942 | OW | WAT | 613 | 11.410  | 46.061 | 15.908  | 1.00 | 30.96 |
| ATOM | 2943 | OW | WAT | 614 | 1.890   | 53.075 | 0.396   | 1.00 | 35.43 |
| ATOM | 2944 | OW | WAT | 615 | 14.858  | 54.460 | -19.563 | 1.00 | 36.48 |
| ATOM | 2945 | OW | WAT | 616 | 27.164  | 22.302 | 9.178   | 1.00 | 28.96 |
| ATOM | 2946 | OW | WAT | 617 | 25.844  | 30.643 | 13.373  | 1.00 | 37.70 |
| ATOM | 2947 | OW | WAT | 618 | -11.773 | 30.992 | 19.536  | 1.00 | 35.27 |
| ATOM | 2948 | OW | WAT | 619 | 20.068  | 54.715 | -26.556 | 1.00 | 30.61 |
| ATOM | 2949 | OW | WAT | 620 | 22.511  | 25.529 | 18.055  | 1.00 | 39.02 |
| ATOM | 2950 | OW | WAT | 621 | 4.762   | 24.578 | 19.147  | 1.00 | 29.70 |
| ATOM | 2951 | OW | WAT | 622 | -5.809  | 31.212 | -7.251  | 1.00 | 38.52 |
| ATOM | 2952 | OW | WAT | 623 | 2.302   | 46.734 | -19.134 | 1.00 | 31.35 |
| ATOM | 2953 | OW | WAT | 624 | -3.267  | 26.845 | -9.657  | 1.00 | 26.55 |
| ATOM | 2954 | OW | WAT | 625 | 20.942  | 19.909 | 15.987  | 1.00 | 30.93 |
| ATOM | 2955 | OW | WAT | 626 | 14.335  | 19.417 | 27.897  | 1.00 | 41.36 |
| ATOM | 2956 | OW | WAT | 627 | -8.960  | 44.991 | 2.623   | 1.00 | 32.33 |
| ATOM | 2957 | OW | WAT | 628 | -2.896  | 18.495 | 3.945   | 1.00 | 33.15 |
| ATOM | 2958 | OW | WAT | 629 | 19.081  | 15.066 | 19.313  | 1.00 | 41.85 |
| ATOM | 2959 | OW | WAT | 630 | 26.583  | 40.965 | -16.598 | 1.00 | 53.36 |
| ATOM | 2960 | OW | WAT | 631 | 9.201   | 30.845 | -29.283 | 1.00 | 26.67 |
| ATOM | 2961 | OW | WAT | 632 | 29.771  | 29.232 | 13.030  | 1.00 | 37.22 |
| ATOM | 2962 | OW | WAT | 633 | -9.063  | 44.258 | 5.485   | 1.00 | 30.64 |
| ATOM | 2963 | OW | WAT | 634 | 36.469  | 24.114 | 2.218   | 1.00 | 34.07 |
| ATOM | 2964 | OW | WAT | 635 | 1.658   | 28.923 | 20.644  | 1.00 | 39.44 |
| ATOM | 2965 | OW | WAT | 636 | -8.637  | 37.196 | -3.769  | 1.00 | 39.41 |
| ATOM | 2966 | OW | WAT | 637 | 9.491   | 43.672 | 18.552  | 1.00 | 34.67 |
| ATOM | 2967 | OW | WAT | 638 | 38.446  | 24.948 | 5.405   | 1.00 | 37.88 |
| ATOM | 2968 | OW | WAT | 639 | 16.362  | 21.306 | -12.437 | 1.00 | 35.82 |
| ATOM | 2969 | OW | WAT | 640 | 11.407  | 51.004 | -0.072  | 1.00 | 31.55 |
| ATOM | 2970 | OW | WAT | 641 | 38.229  | 24.335 | 8.085   | 1.00 | 39.89 |
| ATOM | 2971 | OW | WAT | 642 | 21.655  | 26.806 | 22.131  | 1.00 | 32.81 |
| ATOM | 2972 | OW | WAT | 643 | 16.387  | 22.635 | 23.545  | 1.00 | 35.28 |
| ATOM | 2973 | OW | WAT | 644 | -12.122 | 42.861 | -8.757  | 1.00 | 43.21 |
| ATOM | 2974 | OW | WAT | 645 | -1.768  | 30.006 | 19.108  | 1.00 | 39.03 |
| ATOM | 2975 | OW | WAT | 646 | 31.231  | 36.441 | -7.964  | 1.00 | 40.74 |
| ATOM | 2976 | OW | WAT | 647 | -9.784  | 38.920 | 18.620  | 1.00 | 37.25 |
| ATOM | 2977 | OW | WAT | 648 | -5.666  | 31.659 | 21.328  | 1.00 | 32.24 |
| ATOM | 2978 | OW | WAT | 649 | -2.584  | 54.436 | 0.499   | 1.00 | 42.36 |
| ATOM | 2979 | OW | WAT | 650 | 9.314   | 15.276 | 13.185  | 1.00 | 41.13 |
| ATOM | 2980 | OW | WAT | 651 | 20.108  | 12.329 | 9.346   | 1.00 | 30.57 |
| ATOM | 2981 | OW | WAT | 652 | 28.719  | 20.042 | 8.674   | 1.00 | 30.27 |
| ATOM | 2982 | OW | WAT | 653 | 27.567  | 35.432 | 11.915  | 1.00 | 34.47 |
| ATOM | 2983 | OW | WAT | 654 | 20.822  | 18.155 | 14.214  | 1.00 | 29.75 |
| ATOM | 2984 | OW | WAT | 655 | -1.395  | 25.107 | 7.194   | 1.00 | 42.08 |
| END  |      |    |     |     |         |        |         |      |       |

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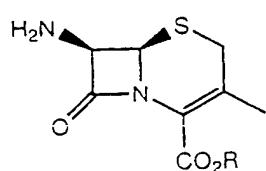
Scheme 1



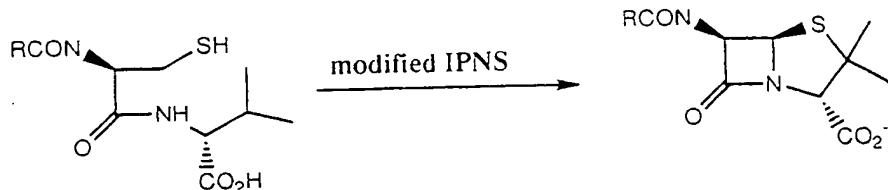
Scheme 2



C-3 exomethylene cephams with hydrophobic side chains, e.g.  
 R = PhCH<sub>2</sub>, R = PhOCH<sub>2</sub>,  
 R = HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub>



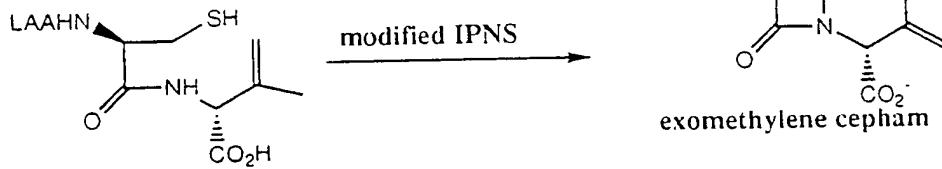
Scheme 5



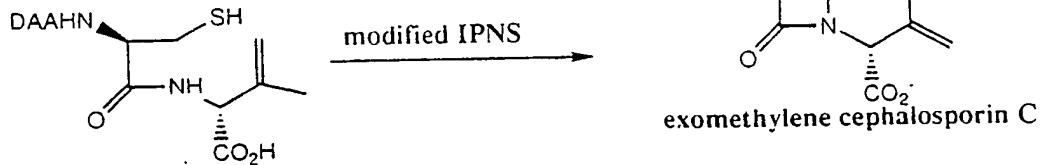
where, R = alkyl or aryl or a combination of both, e.g. PhCH<sub>2</sub>, PhOCH<sub>2</sub>. The alkyl chain or aryl portion of R may also be substituted with acidic or basic groups, e.g. R = HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub>, R = H<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>. R may also be heterocyclic.

Scheme 6

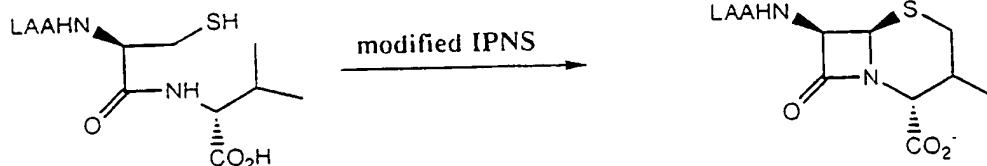
example 1



example 2



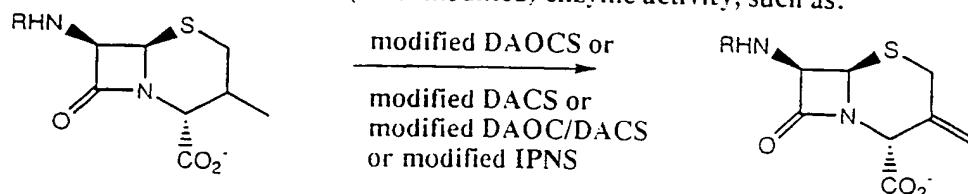
example 3



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Scheme 6 (cont.)

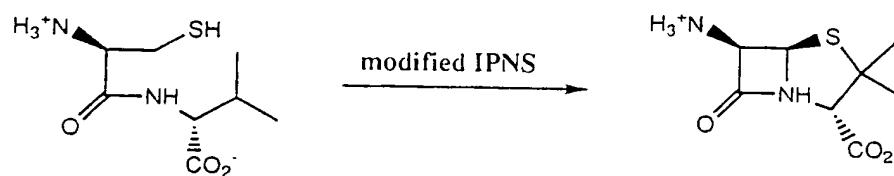
example 3 (cont.) The modified IPNS may be used in conjunction with another modified (or unmodified) enzyme activity, such as:



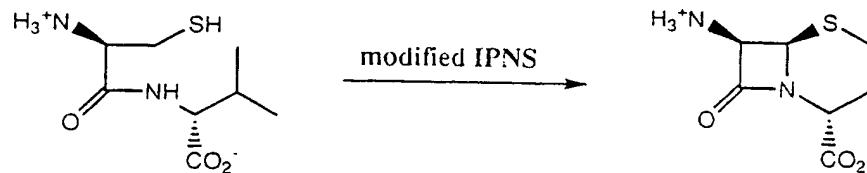
where R = LAA, DAA or other.

Scheme 7

example 1

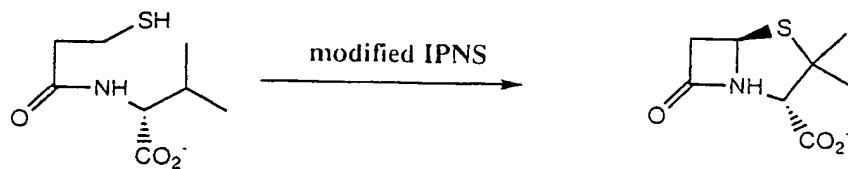


example 2

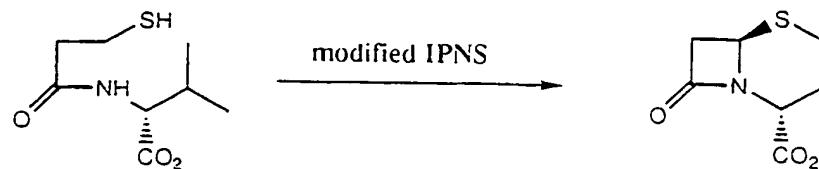


Scheme 8

example 1

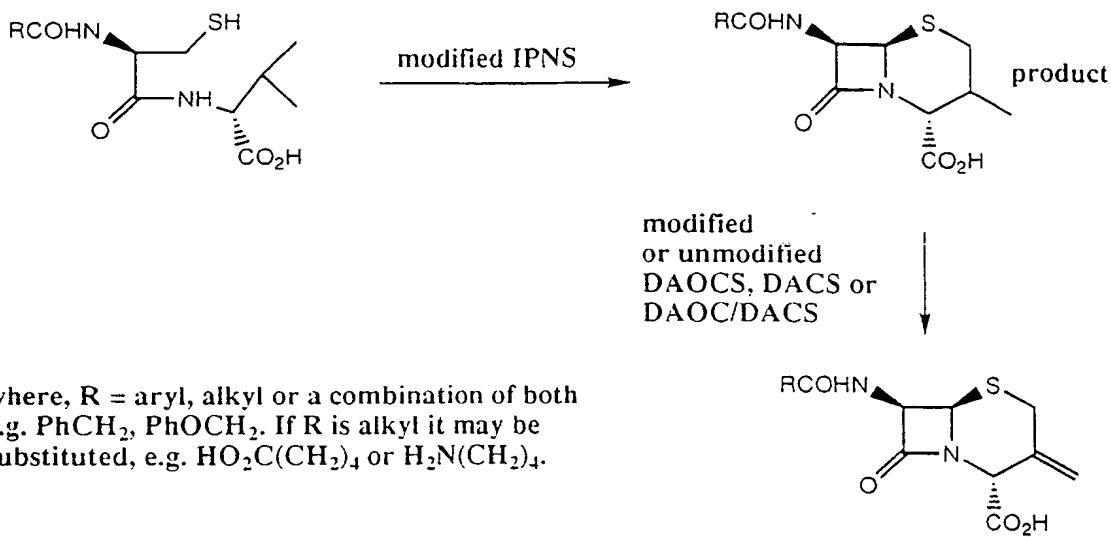


example 2

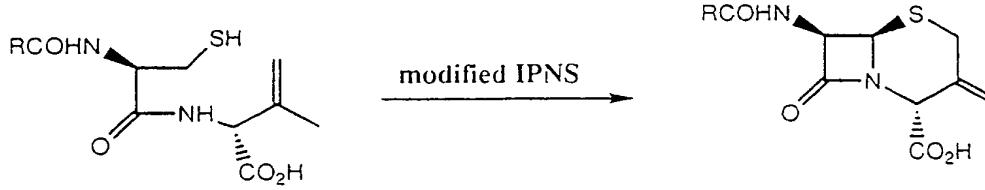


Scheme 9

example 1



example 2

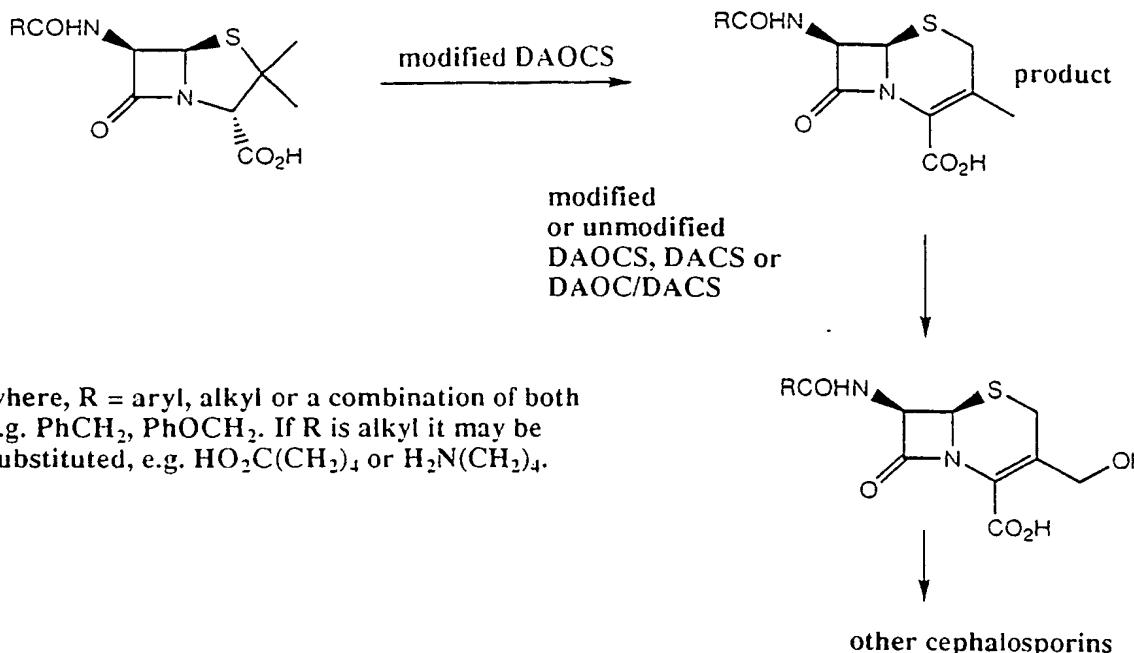


where, R = aryl, alkyl or a combination of both  
e.g. PhCH<sub>2</sub>, PhOCH<sub>2</sub>. If R is alkyl it may be  
substituted, e.g. HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub> or H<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>.  
R = D- $\delta$ -( $\alpha$ -amino adipoyl).

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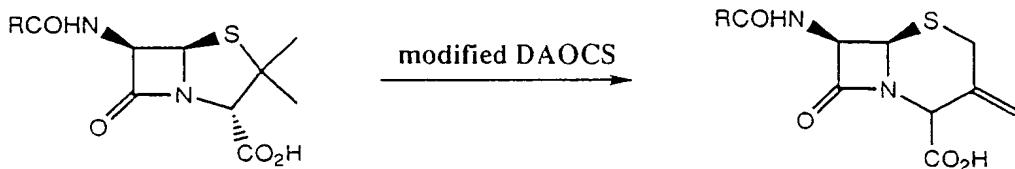
Scheme 10

## examples



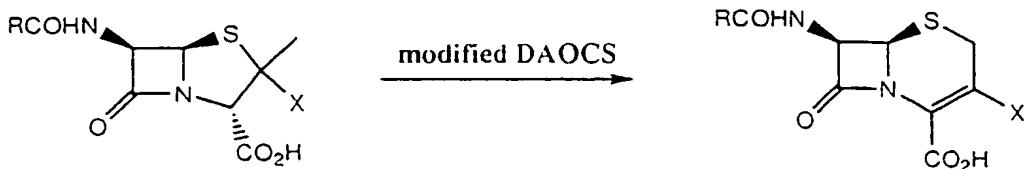
Scheme 11

## example 1



where, R = D- $\delta$ -( $\alpha$ -aminoadipoyl), L- $\delta$ -( $\alpha$ -aminoadipoyl) HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub> or H<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>.

## example 2

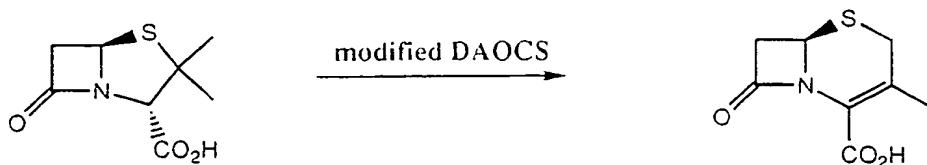


where, R = D- $\delta$ -( $\alpha$ -aminoadipoyl), D- $\delta$ -( $\alpha$ -aminoadipoyl) HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub> or H<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>, X = Cl, Br, I, OMe, SMe, or other substituent.

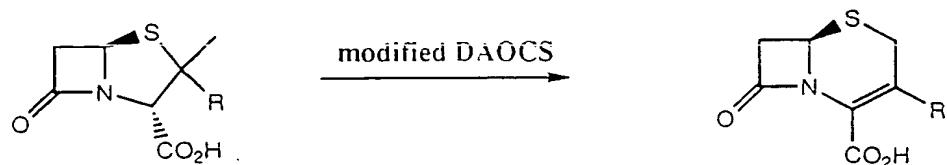
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Scheme 13

example 1



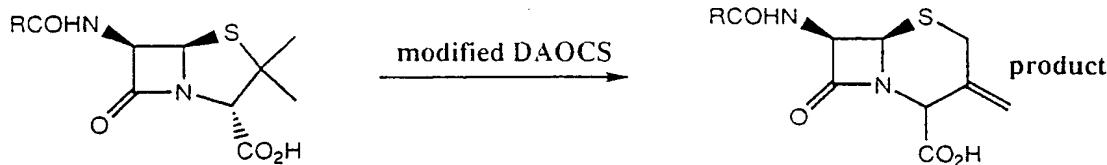
example 2



where R = Cl, Br, I, OMe or other substituent.

Scheme 14

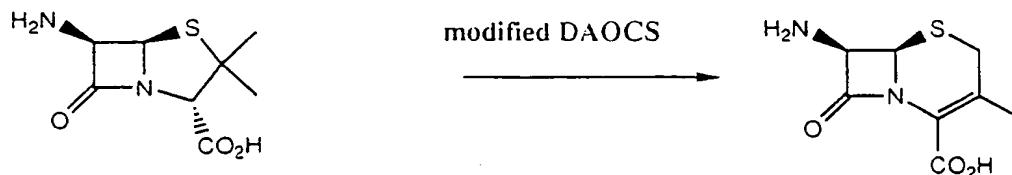
examples



where, R = aryl, alkyl or a combination of aryl and alkyl  
e.g. PhCH<sub>2</sub>, PhOCH<sub>2</sub>.

Scheme 12

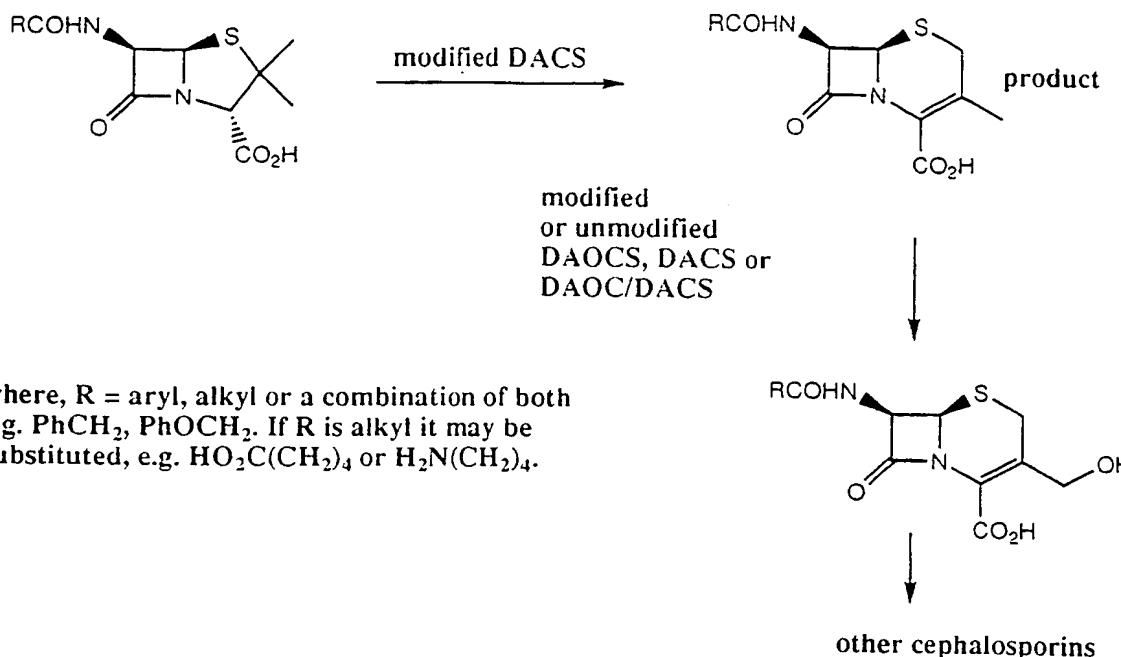
example



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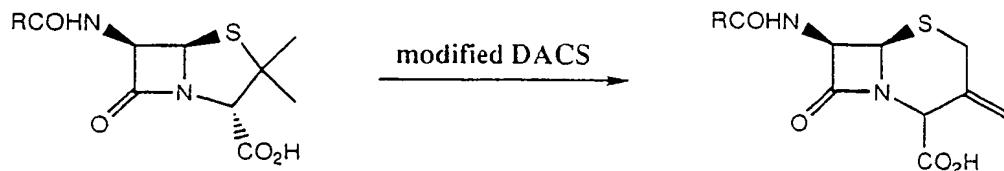
Scheme 15

examples



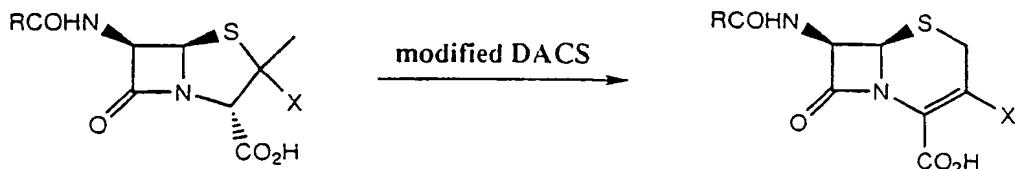
Scheme 16

example 1



where, R = D- $\delta$ -( $\alpha$ -amino adipoyl), L- $\delta$ -( $\alpha$ -amino adipoyl) HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub> or H<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>.

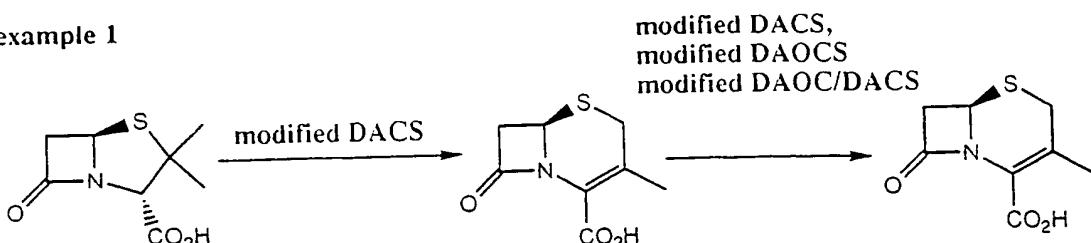
example 2



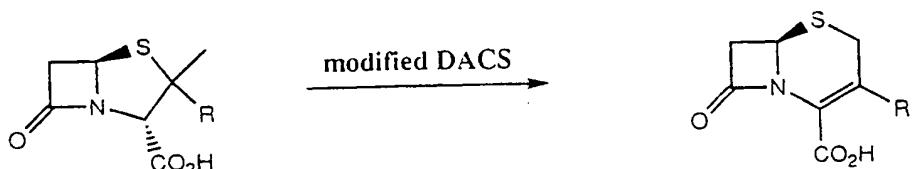
where, R = D- $\delta$ -( $\alpha$ -amino adipoyl), D- $\delta$ -( $\alpha$ -amino adipoyl) HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub> or H<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>, X = Cl, Br, I, OMe, SMe, or other substituent.

Scheme 18

## example 1



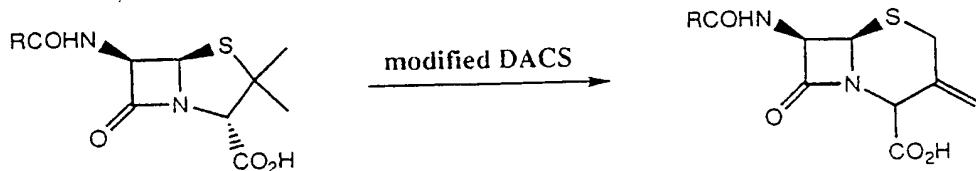
## example 2



where R = Cl, Br, I, OMe or other substituent.

Scheme 19

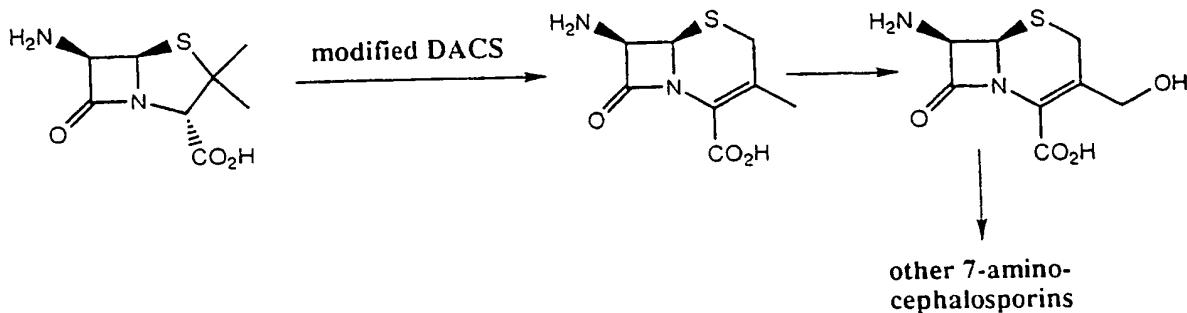
## examples



where, R = aryl, alkyl or a combination of aryl and alkyl  
e.g. PhCH<sub>2</sub>, PhOCH<sub>2</sub>.

Scheme 17

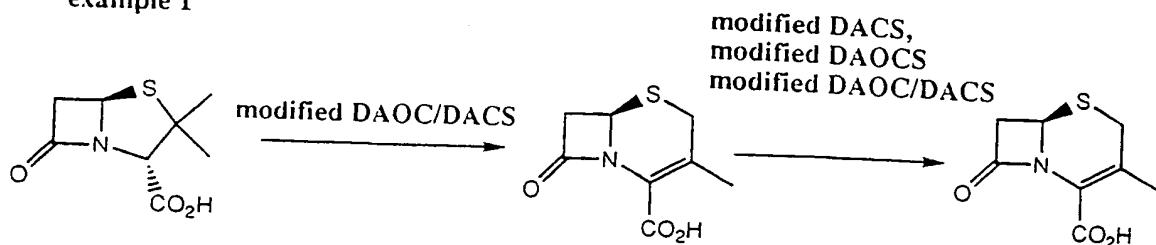
## example



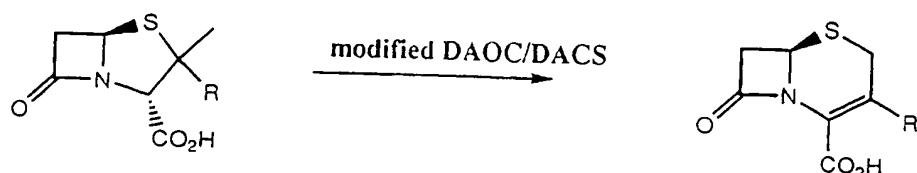
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Scheme 22

## example 1



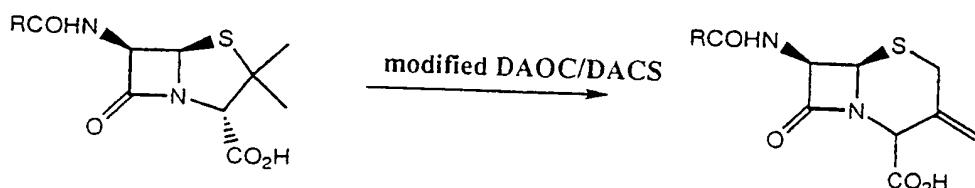
## example 2



where R = Cl, Br, I, OMe or other substituent.

Scheme 23

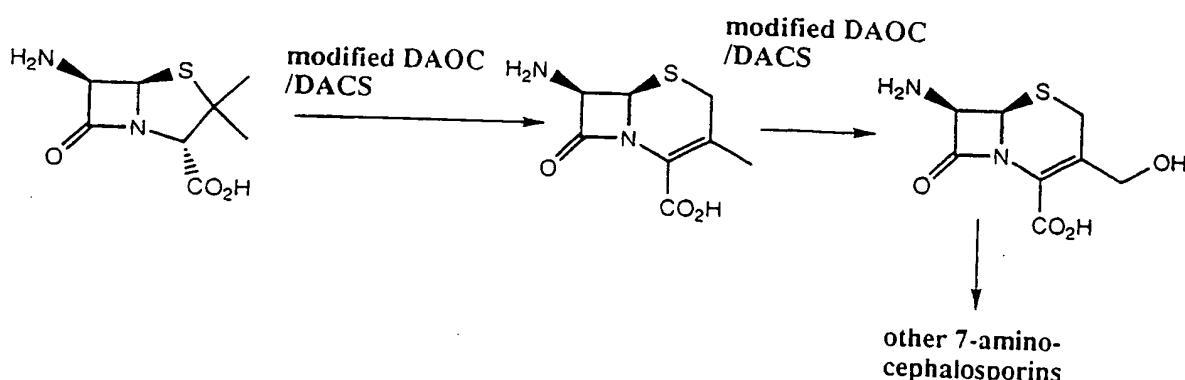
## examples



where, R = aryl, alkyl or a combination of aryl and alkyl  
e.g. PhCH<sub>2</sub>, PhOCH<sub>2</sub>.

Scheme 21

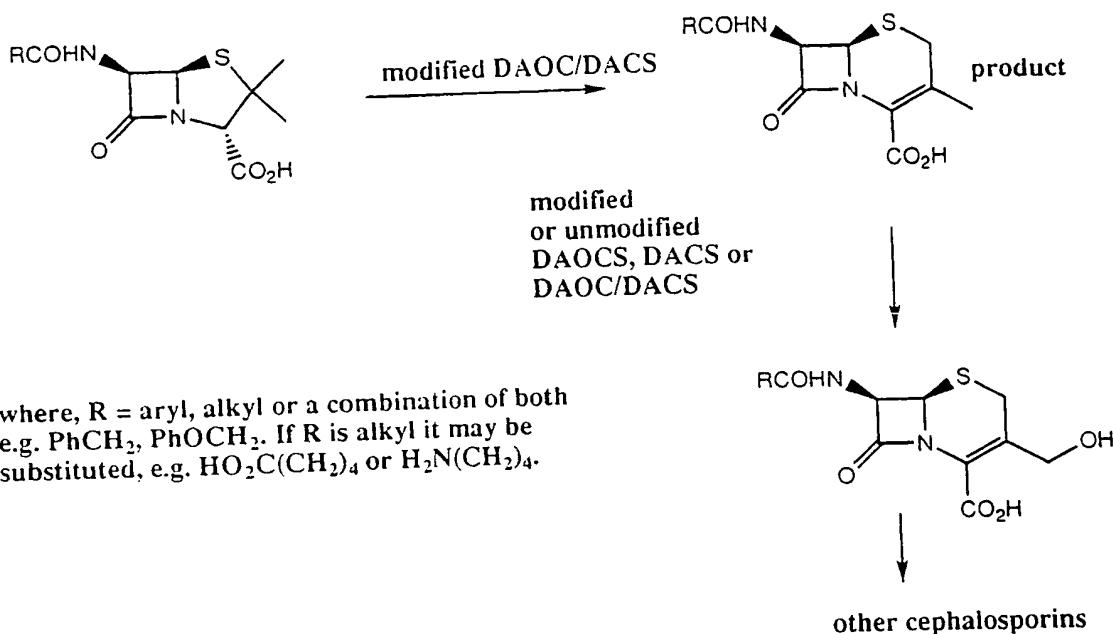
## example



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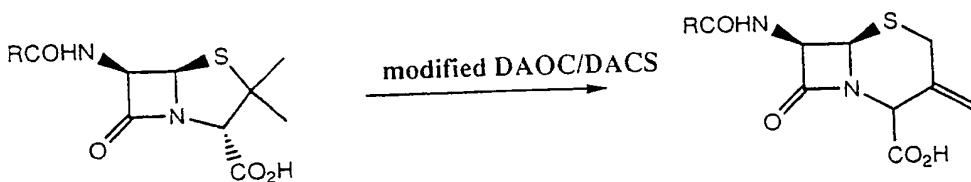
Scheme 24

examples



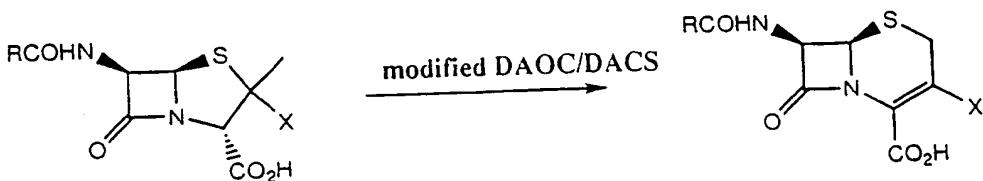
Scheme 20

example 1



where, R = D- $\delta$ -( $\alpha$ -amino adipoyl), L- $\delta$ -( $\alpha$ -amino adipoyl) HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub> or H<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>.

example 2



where, R = D- $\delta$ -( $\alpha$ -amino adipoyl), D- $\delta$ -( $\alpha$ -amino adipoyl) HO<sub>2</sub>C(CH<sub>2</sub>)<sub>4</sub> or H<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>, X = Cl, Br, I, OMe, SMe, or other substituent.

CLAIMS

5 1. Isopenicillin N synthase (IPNS) in the form of: a complex with Mn having a structure designated by the X-ray co-ordinates in Table 2; or a complex with Fe and its substrate, said complex having a structure designated by the X-ray co-ordinates in Table 3.

10 2. Isopenicillin N synthase (IPNS) in the form of: a complex with Fe and an analogue of its substrate, either in the absence or in the presence of nitrous oxide or dioxygen, said complex having a structure designated by X-ray co-ordinates analogous to that set out in Table 3.

15 3. Use of the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for the modification of a second enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway.

20 4. Use as claimed in claim 3, wherein the second enzyme is modified to accept unnatural substrates for the preparation of antibacterial materials or intermediate for the production of pharmaceutical products.

5. Use as claimed in claim 3, wherein the second enzyme is modified to produce unnatural products or improve the production of natural products.

25 6. An enzyme having significant (as herein defined) sequence similarity to IPNS, wherein at least one of the following amino acid residues is modified:

R287; R87; R88; Y189; S183; Y91; F285; Q330; T331;  
V185; L106; C104; V217; L324; L317; I325; L321; S210.

7. An enzyme having significant (as herein defined) sequence similarity to IPNS, wherein at least one of the following amino acid residues is modified:  
V272; L231; L223; P283; T221; F211; F285; Q330;  
5 I187; V185; Y189; R279; S281; N230; Q225; N252; S210.
8. A gene which codes for the enzyme of claim 6 or claim 7.
9. A micro-organism containing the gene of claim 8 and which is capable of expressing the gene under fermentation conditions.
10. Use of the micro-organism of claim 9 for making a bicyclic  $\beta$ -lactam of the penicillin or cephalosporin (including cephams) families.
11. Use of the enzyme of claim 6 or claim 7 for the preparation *in vitro* of a bicyclic  $\beta$ -lactam of the penicillin and cephalosporin families.
12. In a method for the preparation of an enzyme, selected from IPNS, DAOCS, DACS, DAOC/DACS and sequence-related enzymes, in crystalline form for X-ray diffraction studies, the improvement which consists in maintaining the enzyme under anaerobic conditions with dioxygen substantially absent.
13. A method which comprises using the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for determining or predicting the structure of a second enzyme which is structurally related to the first enzyme but is not active in the penicillin or cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the 20 second enzyme or for designing an inhibitor for the second enzyme.
14. Use of the enzyme of claim 6 or claim 7 to convert a dipeptide to a 6- aminopenicillin or other bicyclic  $\beta$ -lactam.
15. Use as claimed in claim 14, wherein the dipeptide has been produced by use of a peptide synthetase enzyme such as ACV synthetase 30 optionally modified to optimise dipeptide production.





## INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

|   |  |  |  |
|---|--|--|--|
| (51) International Patent Classification 6 :<br><br>C12N 15/52, 9/00, C12P 35/00, C12N 1/21   |  | A3   | (11) International Publication Number: <b>WO 98/16648</b><br><br>(43) International Publication Date: 23 April 1998 (23.04.98) |
| <p>(21) International Application Number: PCT/GB97/02838</p> <p>(22) International Filing Date: 15 October 1997 (15.10.97)</p> <p>(30) Priority Data:<br/>9621486.1 15 October 1996 (15.10.96) GB</p> <p>(71) Applicant (for all designated States except US): ISIS INNOVATION LIMITED [GB/GB]; 2 South Parks Road, Oxford OX1 3UB (GB).</p> <p>(72) Inventors; and</p> <p>(75) Inventors/Applicants (for US only): SCHOFIELD, Christopher, Joseph [GB/GB]; 19 Delamare Way, Cumnor Hill, Oxford OX2 9HZ (GB). BALDWIN, Jack, Edward [GB/GB]; Broom, Hinksey Hill, Oxford OX1 5BH (GB). CLIFTON, Ian [GB/GB]; 1 Staincross House, Albion Place, Oxford OX1 1SG (GB). HAJDU, Janos [HU/SE]; Stabby Malmsvagen 8, S-755 91 Uppsala (SE). HENSGENS, Charles [NL/NL]; Oscar Wildestraat 7, NL-9746 AR Groningen (NL). ROACH, Peter, Lawrence [GB/GB]; Exeter College, Oxford OX1 3DP (GB).</p> <p>(74) Agent: PENNANT, Pyers; Stevens Hewlett &amp; Perkins, 1 Serjeants Inn, Fleet Street, London EC4Y 1LL (GB).</p> |  | <p>(81) Designated States: JP, US, European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE).</p> <p><b>Published</b><br/><i>With international search report.<br/>Before the expiration of the time limit for amending the claims and to be republished in the event of the receipt of amendments.</i></p> <p>(88) Date of publication of the international search report: 13 August 1998 (13.08.98)</p> |  |
| <p>(54) Title: ISOPENICILLIN N SYNTHETASE AND DEACETOXYCEPHALOSPORIN C SYNTHETASE ENZYMES AND METHODS</p> <p>(57) Abstract</p> <p>A three-dimensional structure is described of a complex of isopenicillin N synthase (IPNS) with Fe and its substrate ACV. This structure is used to design modified enzymes IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, which modified enzymes may accept unnatural substrates or improve production efficiency or produce improved products. Specific modifications of specific amino acid residues are proposed and exemplified.</p>   |  |  |  |

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## INTERNATIONAL SEARCH REPORT

International Application No  
PCT/GB 97/02838A. CLASSIFICATION OF SUBJECT MATTER  
IPC 6 C12N15/52 C12N9/00 C12P35/00 C12N1/21

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)  
IPC 6 C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category <sup>a</sup> | Citation of document, with indication, where appropriate, of the relevant passages  | Relevant to claim No. |
|-----------------------|---|-----------------------|
| X                     | ROACH PL ET AL: "Crystal structure of isopenicillin N synthase is the first from a new structural family of enzymes."<br>NATURE 375 (6533) P700-4 JUN 22 1995,<br>XP002059796<br>cited in the application<br>see abstract; figures 1-3; table 1<br>---                                    | 1                     |
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 Further documents are listed in the continuation of box C. Patent family members are listed in annex.

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Date of the actual completion of the international search

11 June 1998

Date of mailing of the international search report

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## INTERNATIONAL SEARCH REPORT

Serial Application No  
PCT/GB 97/02838

## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

| Category | Citation of document, with indication, where appropriate, of the relevant passages   | Relevant to claim No.  |
|----------|--|------------------------|
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|          |  | -/-                    |

## INTERNATIONAL SEARCH REPORT

International Application No  
PCT/GB 97/02838

## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

| Category | Citation of document, with indication, where appropriate, of the relevant passages   | Relevant to claim No.  |
|----------|--|------------------------|
| A        | <p>TAN, DOREEN S. H. ET AL: "Functional analysis of conserved histidine residues in <i>Cephalosporium acremonium</i> isopenicillin N synthase by site-directed mutagenesis" <i>J. BIOL. CHEM.</i> (1996), 271(2), 889-94 CODEN: JBCHA3; ISSN: 0021-9258, XP002060004</p> <p>see abstract</p> <p>see page 889, right-hand column, paragraph 2; figures 1,4; tables 2,3</p> <p>see page 893, left-hand column, paragraph 2</p> <p>---</p>  | 1,2,<br>6-11,14,<br>15 |
| A        | <p>KRIAUCIUNAS A ET AL: "The functional role of cysteines in isopenicillin N synthase. Correlation of cysteine reactivities toward sulphydryl reagents with kinetic properties of cysteine mutants." <i>J BIOL CHEM</i>, JUN 25 1991, 266 (18) P11779-88, UNITED STATES, XP002060005</p> <p>see abstract</p> <p>see page 11780, left-hand column, paragraph 3</p> <p>see page 11782, right-hand column, line 12 - line 17</p> <p>---</p> | 1,2,<br>6-11,14,<br>15 |
| P,X      | <p>SAMI, MALKIT ET AL: "Glutamine-330 is not essential for activity in isopenicillin N synthase from <i>Aspergillus nidulans</i>" <i>FEBS LETT.</i> (1997), 405(2), 191-194 CODEN: FEBLAL; ISSN: 0014-5793, XP002059797</p> <p>see the whole document</p> <p>---</p>   | 1,6-11,<br>14,15       |
| P,X      | <p>ROACH, PETER L. ET AL: "Structure of isopenicillin N synthase complexed with substrate and the mechanism of penicillin formation" <i>NATURE (LONDON)</i> (1997), 387(6635), 827-830 CODEN: NATUAS; ISSN: 0028-0836, XP002067787</p> <p>see the whole document</p> <p>---</p>  | 1,2                    |
| P,X      | <p>WO 97 20053 A (GIST BROCADES BV ;UNIV OXFORD (GB); SUTHERLAND JOHN DAVID (GB); BO) 5 June 1997</p> <p>see claims 1-9; figure 1</p> <p>-----</p>   | 6-11,14,<br>15         |

# INTERNATIONAL SEARCH REPORT

II. International application No.  
PCT/GB 97/02838

## Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1.  Claims Nos.: because they relate to subject matter not required to be searched by this Authority, namely:
  
2.  Claims Nos.: because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
  
3.  Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

## Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see additional sheet

1.  As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
  
2.  As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
  
3.  As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:

1 2 6-11 14 15

4.  No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

### Remark on Protest

The additional search fees were accompanied by the applicant's protest.

No protest accompanied the payment of additional search fees.

# INTERNATIONAL SEARCH REPORT

International Application No. PCT/GB 97/02838

## FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. Claim : 1 partly

IPNS complexed with Mn

2. Claim : 2 and 1 partly

IPNS complexed with Fe and 1st substrate or an analogue of its substrate

3. Claims: 3-5 , 13

the use of the three dimensional structure of a member of the IPNS family of enzymes to modify another enzyme .

4. Claims: 6-11,14-15

Enzyme having significant sequence similarity to IPNS wherein at least one of the following amino acid residues is modified ,r87,y189,s183,y91,f285,q330,t331,v185,l106,c104,v217,1324,1317,i325,i321,s210,v272,l231,1223,p283,t221,f211,i187,v185,y189,r279,s281,n230,q225,n252,r287,r88, mutants of an enzyme having similarity to IPNS , gene encoding it , micro-organism containing the gene and their use in beta-lactam production .

5. Claim : 12

methods of preparation of an enzyme of the IPNS family in crystalline form consisting of maintaining the crystalline enzymes of the IPNS family under anaerobic conditions .

## INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/GB 97/02838

| Patent document cited in search report | Publication date | Patent family member(s) |         |   | Publication date |
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